Nonclassical Transport Theory and Applications

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My research interests

Mathematical Modeling

Particle transport and diffusion processes

Computational Modeling

Deterministic methods; Monte Carlo methods; hybrid methods

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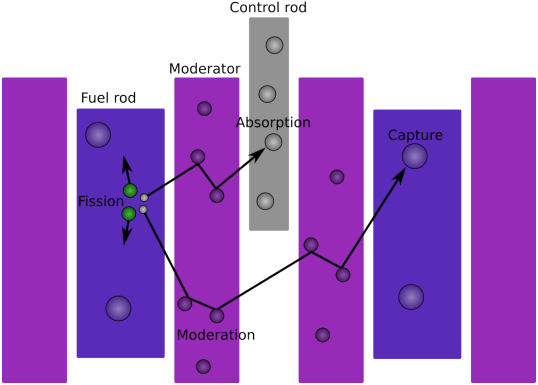
Tools for Real Problems!

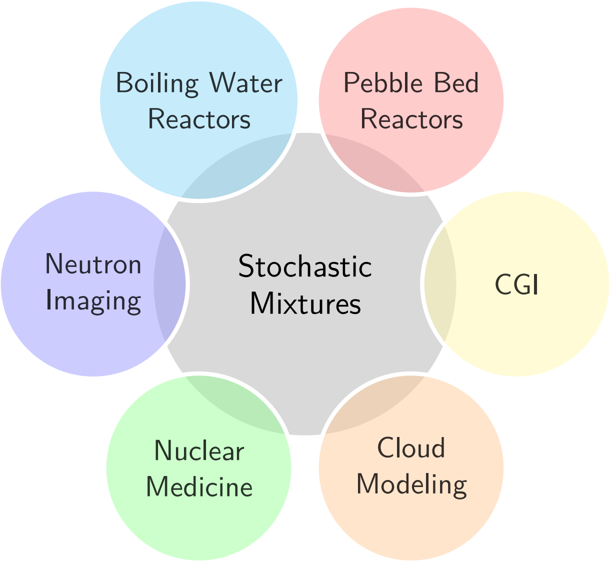
Heterogeneous systems

If the geometry of the background medium is known...

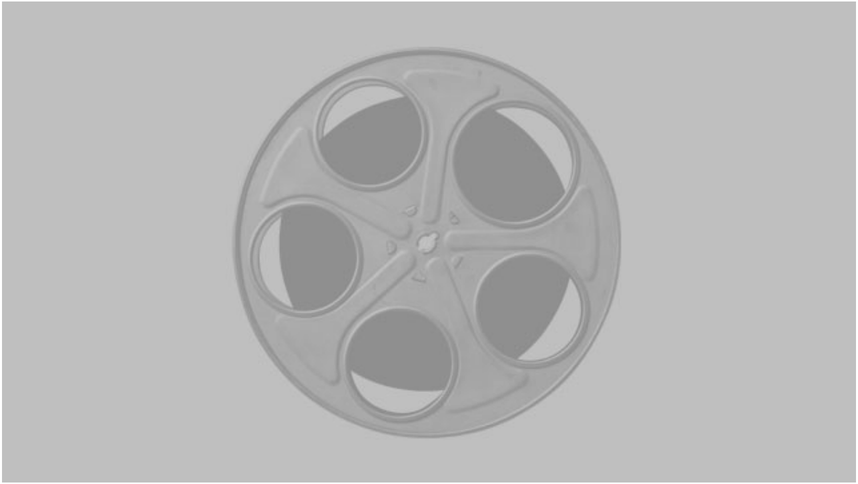
... it is fairly straightforward to define the parameters of the material in space.



Heterogeneous systems



Example: PBR



*Movie by Chris H. Rycroft

Modeling transport in stochastic media

Goal

To obtain an accurate estimate for the *ensembled-averaged* flux.

- "Brute Force" approach
  - Simulate a large number of physical realizations of the system
- Coupling models
  - Levermore-Pomraning Equations*

*Journal of Quantitative Spectroscopy & Radiative Transfer 154, 2015

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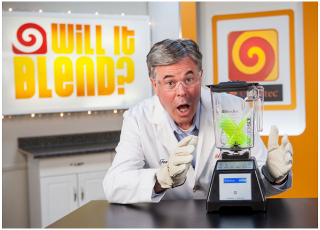
- Coupling models
  - Levermore-Pomraning Equations*
- Homogenization techniques



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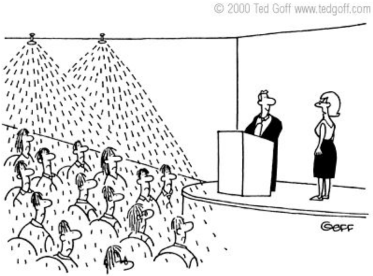
Outline

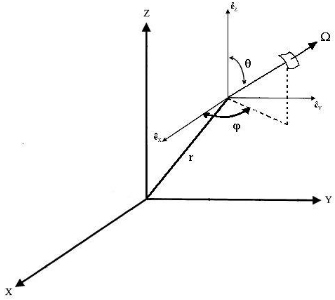


"You're not allowed to use the sprinkler system to keep your audience awake."

- Classical transport and homogenization
- Nonclassical transport
- Formulations
- Results
- Synergies and the future

What we want

Given a standard transport process in time t, we want to be able to estimate the number of particles that....



- ... are located at the spatial point $\boldsymbol{x}$
- ... are traveling in the direction $\boldsymbol{\Omega}$
- ... have energy E

In other words, we want an expression for the *angular flux*:

$$\psi(\boldsymbol{x}, \boldsymbol{\Omega}, E, t)$$

The steady-state linear Boltzmann equation

$$\overbrace{\boldsymbol{\Omega}\cdot\nabla\psi(\boldsymbol{x},\boldsymbol{\Omega})}^{\text{Leakage}} + \overbrace{\Sigma_t(\boldsymbol{x})\psi(\boldsymbol{x},\boldsymbol{\Omega})}^{\text{Absorption+Out-scattering}} = \underbrace{\frac{c(\boldsymbol{x})\Sigma_t(\boldsymbol{x})}{4\pi}\int_{4\pi}\psi(\boldsymbol{x},\boldsymbol{\Omega}')d\Omega'}_{\text{In-scattering}} + \underbrace{\frac{Q(\boldsymbol{x})}{4\pi}}_{\text{Source}}$$

- The **total cross-section** Σ_t is defined such that $\Sigma_t ds$ represents the probability that a particle will collide when traveling an incremental distance ds
- The **scattering ratio** c is the probability that a collided particle will scatter
- Scattering is assumed to be **isotropic**
- The source Q emits particles **isotropically**
- Transport is **monoenergetic**

Homogenization: the Atomic Mix model

The atomic mix model homogenizes the medium by **volume-averaging the parameters**.

Let $p_i(\boldsymbol{x})$ be the probability of finding material i at spatial point $\boldsymbol{x}$; then

- $\langle \Sigma_t \rangle(\boldsymbol{x}) = p_1(\boldsymbol{x})\Sigma_{t,1} + p_2(\boldsymbol{x})\Sigma_{t,2}$
- $\langle c\Sigma_t \rangle(\boldsymbol{x}) = p_1(\boldsymbol{x})c_1\Sigma_{t,1} + p_2(\boldsymbol{x})c_2\Sigma_{t,2}$
- $\langle Q \rangle(\boldsymbol{x}) = p_1(\boldsymbol{x})Q_1 + p_2(\boldsymbol{x})Q_2$

Assuming the statistics of the mixture to be homogeneous, the $\boldsymbol{x}$-dependence can be dropped

The Atomic Mix equation

Transport equation

$$\boldsymbol{\Omega} \cdot \nabla \psi(\boldsymbol{x}, \boldsymbol{\Omega}) + \Sigma_t(\boldsymbol{x}) \psi(\boldsymbol{x}, \boldsymbol{\Omega}) = \frac{c(\boldsymbol{x})\Sigma_t(\boldsymbol{x})}{4\pi} \int_{4\pi} \psi(\boldsymbol{x}, \boldsymbol{\Omega}') d\Omega' + \frac{Q(\boldsymbol{x})}{4\pi}$$

Atomic Mix Equation

$$\boldsymbol{\Omega} \cdot \nabla \left\langle \psi \right\rangle(\boldsymbol{x}, \boldsymbol{\Omega}) + \left\langle \Sigma_t \right\rangle \left\langle \psi \right\rangle(\boldsymbol{x}, \boldsymbol{\Omega}) = \frac{\left\langle c\Sigma_t \right\rangle}{4\pi} \int_{4\pi} \left\langle \psi \right\rangle(\boldsymbol{x}, \boldsymbol{\Omega}') d\Omega' + \frac{\left\langle Q \right\rangle}{4\pi}$$

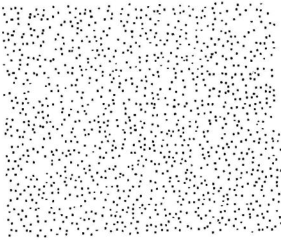
+ Simplicity of model
+ No extra work needed to implement it
+ Accurate when “chunks” of each material are optically thin*

- Terribly inaccurate when the “chunks" are optically thick
- Resulting flux is a “black box"
- Does not preserve important physical aspects of certain types of systems

*Proceedings of M&C 2015, Avignon, France

In classical transport

The "colliders" in the background material are, in general, **Poisson-distributed**; that is, their spatial locations are **not** correlated.



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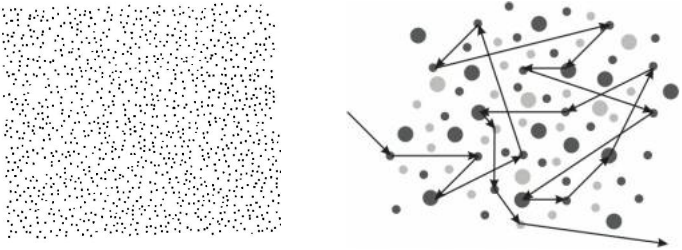
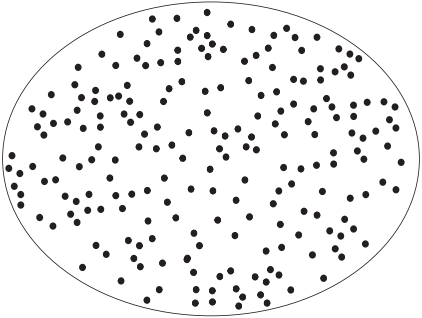


Specifically, this implies that the probability distribution function $p(s)$ for particles' **distances-to-collision** (free-paths) is given by an exponential:

$$p(s) = \Sigma_t e^{-\Sigma_t s}$$

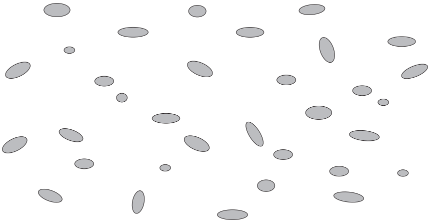
When is transport “nonclassical”?

Consider a large single “clump” of randomly-spaced (uncorrelated) scattering centers. Particles that enter such a clump will undergo many “classical" collisions before exiting.



Random "cloud" system

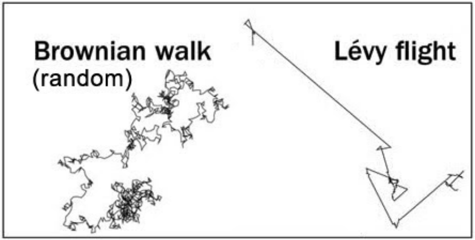
Now consider a much larger system, consisting of many widely-spaced clumps of the above type, all separated by a "void":



Relatively rare events (streaming between clumps) will significantly affect the particle transport. The free-path distribution $p(s)$ will have a **nonexponential peak** for large s.

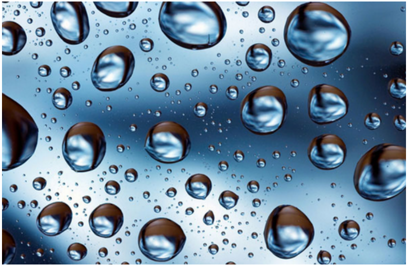
Lévy flights

A Lévy flight is a random walk in which the step-lengths have a probability distribution that is heavy-tailed:



- Lévy glasses
- Astronomy
- Cryptography
- Earthquake data analysis
- Financial mathematics
- Foraging hypothesis

Real-world applications



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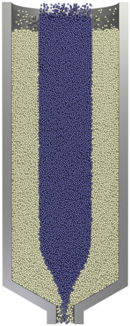

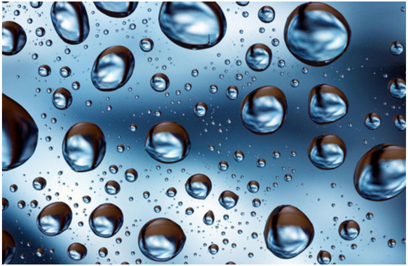

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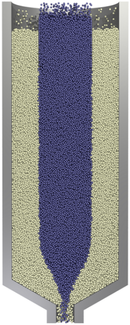

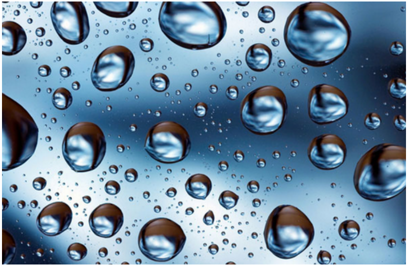

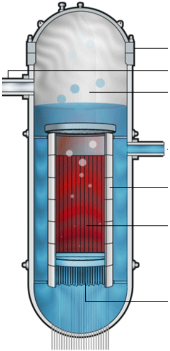

Free-path distribution

In classical particle transport, the incremental probability dp that a particle will experience a collision while traveling an incremental path length ds is:

$$dp = \Sigma_t \, ds \ ,$$

where the total cross section Σ_t is independent of

$$\boxed{s = \text{the path length traveled since the previous interaction} \ .}$$

Assuming that $\Sigma_t = \Sigma_t(s)$, the free-path distribution is given by*

$$\boxed{p(s) = \Sigma_t(s) e^{-\int_0^s \Sigma_t(s') ds'} \ .}$$

In classical transport, $p(s) = \Sigma_t e^{-\Sigma_t s} =$ exponential .

* Σ_t can also depend on $\boldsymbol{\Omega}$ (Annals of Nuclear Energy 70, 2014)

The nonclassical linear Boltzmann equation

Nonclassical transport

$$\frac{\partial\psi}{\partial s}(\boldsymbol{x},\boldsymbol{\Omega},s) + \boldsymbol{\Omega}\cdot\boldsymbol{\nabla}\psi(\boldsymbol{x},\boldsymbol{\Omega},s) + \Sigma_t(s)\psi(\boldsymbol{x},\boldsymbol{\Omega},s) = \frac{\delta(s)}{4\pi}\left[c\int_{4\pi}\int_0^\infty \Sigma_t(s')\psi(\boldsymbol{x},\boldsymbol{\Omega}',s')\,ds'\,d\Omega' + Q(\boldsymbol{x})\right]$$

Classical transport

$$\boldsymbol{\Omega}\cdot\nabla\psi(\boldsymbol{x},\boldsymbol{\Omega}) + \Sigma_t\psi(\boldsymbol{x},\boldsymbol{\Omega}) = \frac{1}{4\pi}\left[c\Sigma_t\int_{4\pi}\psi(\boldsymbol{x},\boldsymbol{\Omega}')d\Omega' + Q(\boldsymbol{x})\right]$$

Integral equation formulation

$$f(\boldsymbol{x}) = \int\int\int [cf(\boldsymbol{x}') + Q(\boldsymbol{x}')]\frac{p(|\boldsymbol{x}'-\boldsymbol{x}|)}{4\pi|\boldsymbol{x}'-\boldsymbol{x}|^2}dV'$$

where $f(\boldsymbol{x}) = \int_0^\infty \int_{4\pi} \Sigma_t(s)\psi(\boldsymbol{x},\boldsymbol{\Omega},s)d\Omega ds = \text{collision-rate density}$

We can use the integral formulation to find representations of classical models. All we need to do is find the correct $p(s)$.

If $p(s) = \Sigma_t e^{-\Sigma_t s}$, we obtain **classical transport**.

If $p(s) = 3\Sigma_t^2 s e^{-\sqrt{3}\Sigma_t s}$, we obtain **classical diffusion**.

This can be extended to the simplified spherical harmonics (SP_N) equations* and to nonclassical diffusion**.

*SIAM Journal on Applied Mathematics 75, 2015

**Applied Mathematics Letters 53, 2016

Diffusion models as asymptotic limits

We can derive a nonclassical diffusion equation using asymptotic analysis*:

Nonclassical diffusion

$$-\frac{1}{6}\frac{\langle s^2\rangle}{\langle s\rangle}\nabla^2\phi(\boldsymbol{x}) + \frac{(1-c)}{\langle s\rangle}\phi(\boldsymbol{x}) = Q(\boldsymbol{x}).$$

Classical diffusion

$$-\frac{1}{3\Sigma_t}\nabla^2\phi(\boldsymbol{x}) + (1-c)\Sigma_t\phi(\boldsymbol{x}) = Q(\boldsymbol{x}).$$

Moreover, nonclassical SP_N equations can also be asymptotically derived**.

*Journal of Quantitative Spectroscopy and Radiative Transfer 112, 2011
**arXiv:1610.04314 [nucl-th] (M&C 2017)

Numerical results: diffusive PBR system*

Table 7: Diffusion coefficients in random structures

Problem		Monte Carlo		Atomic Mix and Corrections			"Old" GLBE	New GLBE	
		D_x^{mc}	D_z^{mc}	D^{am}	D^B	D^L	D^{iso}	D_x^{gt}	D_z^{gt}
1	Diffusion Coeff.	0.6144	0.6157	0.5617	0.6009	0.5990	0.6147	0.6146	0.6150
	error_x (%)	-	-	8.580	2.201	2.506	0.049	0.029	-
	error_z (%)	-	-	8.776	2.411	2.716	0.166	-	0.126
2	Diffusion Coeff.	0.3286	0.3295	0.2809	0.3200	0.3214	0.3326	0.3324	0.3329
	error_x (%)	-	-	14.542	2.617	2.214	1.204	1.154	-
	error_z (%)	-	-	14.771	2.877	2.475	0.934	-	1.034

*Annals of Nuclear Energy 70, 2014

The nonclassical linear Boltzmann equation

Nonclassical transport

$$\frac{\partial\psi}{\partial s}(\boldsymbol{x},\boldsymbol{\Omega},s) + \boldsymbol{\Omega}\cdot\boldsymbol{\nabla}\psi(\boldsymbol{x},\boldsymbol{\Omega},s) + \Sigma_t(s)\psi(\boldsymbol{x},\boldsymbol{\Omega},s) = \frac{\delta(s)}{4\pi}\left[c\int_{4\pi}\int_0^\infty \Sigma_t(s')\psi(\boldsymbol{x},\boldsymbol{\Omega}',s')\,ds'\,d\Omega' + Q(\boldsymbol{x})\right]$$

Classical transport

$$\boldsymbol{\Omega}\cdot\nabla\psi(\boldsymbol{x},\boldsymbol{\Omega}) + \Sigma_t\psi(\boldsymbol{x},\boldsymbol{\Omega}) = \frac{1}{4\pi}\left[c\Sigma_t\int_{4\pi}\psi(\boldsymbol{x},\boldsymbol{\Omega}')d\Omega' + Q(\boldsymbol{x})\right]$$

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$\Sigma_t(s) =$ 

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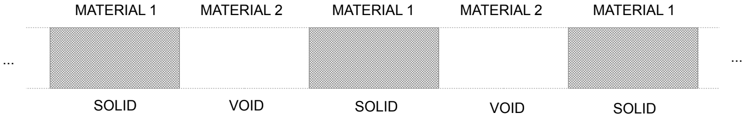
$\Sigma_t(s) =$ 

$$\Sigma_t(s) = \frac{p(s)}{1 - \int_0^s p(s')ds'}$$

1-D random periodic media

We consider a 1-D physical system consisting of alternating layers of solid and void, periodically arranged:



- layers of material 1 and 2 have thicknesses ℓ_1 and ℓ_2, respectively; (period $\ell = \ell_1 + \ell_2$)
- the origin ($x = 0$) is *randomly placed* in the periodic system (this is equivalent to randomly placing the system in the infinite line $-\infty < x < \infty$)
- the probability P_i of finding material i in a given point x is $\ell_i/(\ell_1 + \ell_2)$

The free-path distribution function

The cross sections are stochastic functions of space:

$$\Sigma_t(x) = \begin{cases} \Sigma_{t1}, & \text{if } x \text{ is in material 1} \\ 0, & \text{if } x \text{ is in material 2} \end{cases}$$

We need an analytical expression for

$$p(\mu, s)ds = \begin{array}{l} \text{probability that a particle traveling in the direction } \mu \\ \text{will experience its first collision between } s \text{ and } s + ds \end{array}$$

in the homogenized (ensemble-averaged) material.

- Atomic Mix homogenization yields

$$p(s) = \langle \Sigma_t \rangle e^{-\langle \Sigma_t \rangle s} \quad \text{where} \quad \langle \Sigma_t \rangle = \frac{\ell_1 \Sigma_{t1}}{\ell_1 + \ell_2}$$

The free-path distribution function

★ $\ell_1 < \ell_2$:

$$p(\mu, s) = \begin{cases} \frac{\Sigma_{t1}}{\ell_1}(n\ell + \ell_1 - s|\mu|)e^{-\Sigma_{t1}(s - n\ell_2/|\mu|)}, & \text{if } n\ell \leq s|\mu| \leq n\ell + \ell_1 \\ 0, & \text{if } n\ell + \ell_1 \leq s|\mu| \leq n\ell + \ell_2 \\ \frac{\Sigma_{t1}}{\ell_1}(s|\mu| - n\ell + \ell_2)e^{-\Sigma_{t1}[s - (n+1)\ell_2/|\mu|)]}, & \text{if } n\ell + \ell_2 \leq s|\mu| \leq (n+1)\ell \end{cases}$$

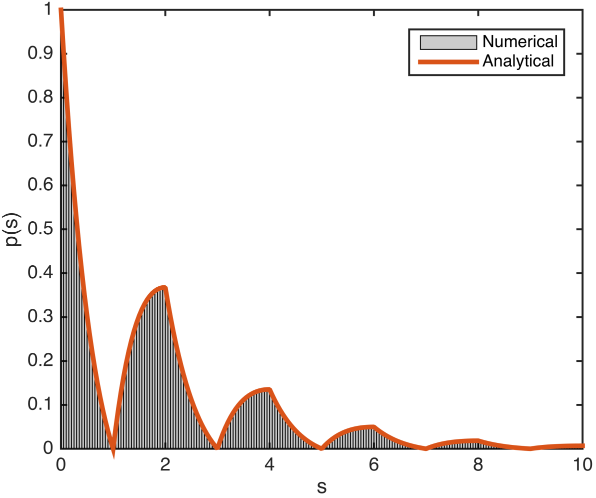
★ $\ell_1 = \ell_2$:

$$p(\mu, s) = \begin{cases} \frac{\Sigma_{t1}}{\ell_1}(n\ell + \ell_1 - s|\mu|)e^{-\Sigma_{t1}(s - n\ell_2/|\mu|)}, & \text{if } n\ell \leq s|\mu| \leq n\ell + \ell_1 \\ \frac{\Sigma_{t1}}{\ell_1}(s|\mu| - n\ell + \ell_2)e^{-\Sigma_{t1}[s - (n+1)\ell_2/|\mu|)]}, & \text{if } n\ell + \ell_2 \leq s|\mu| \leq (n+1)\ell \end{cases}$$

★ $\ell_1 > \ell_2$:

$$p(\mu, s) = \begin{cases} \frac{\Sigma_{t1}}{\ell_1}(n\ell + \ell_1 - s|\mu|)e^{-\Sigma_{t1}(s - n\ell_2/|\mu|)}, & \text{if } n\ell \leq s|\mu| \leq n\ell + \ell_2 \\ \begin{array}{l} \frac{\Sigma_{t1}}{\ell_1}[(n\ell + \ell_2 - s|\mu|)(1 - e^{\Sigma_{t1}\ell_2/|\mu|}) \\ \qquad\qquad + \ell_1 - \ell_2]e^{-\Sigma_{t1}(s - n\ell_2/|\mu|)} \end{array}, & \text{if } n\ell + \ell_2 \leq s|\mu| \leq n\ell + \ell_1 \\ \frac{\Sigma_{t1}}{\ell_1}(s|\mu| - n\ell + \ell_2)e^{-\Sigma_{t1}[s - (n+1)\ell_2/|\mu|)]}, & \text{if } n\ell + \ell_1 \leq s|\mu| \leq (n+1)\ell \end{cases}$$

$p(\mu = 1, s)$ for $\Sigma_{t1} = 1$, with $\ell_1 = \ell_2 = 1$



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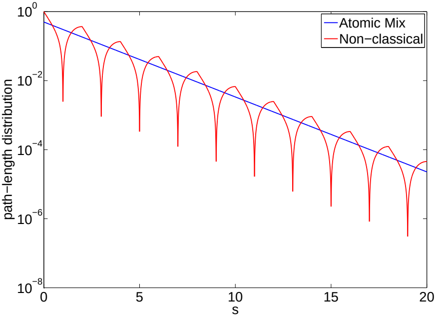

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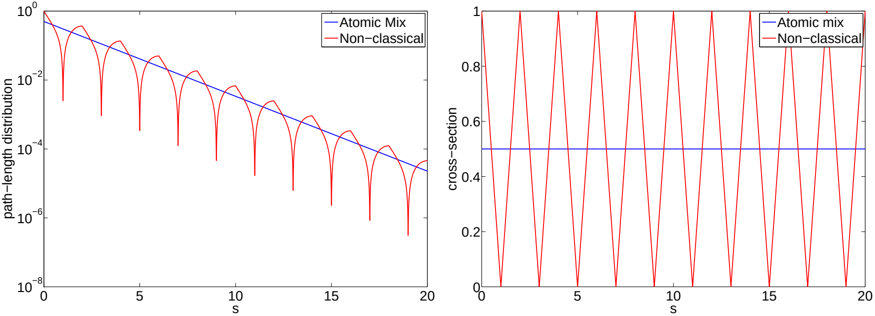
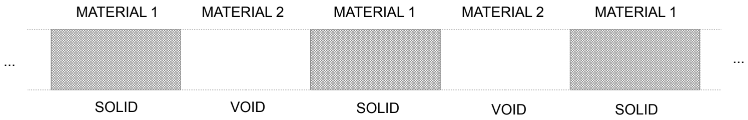


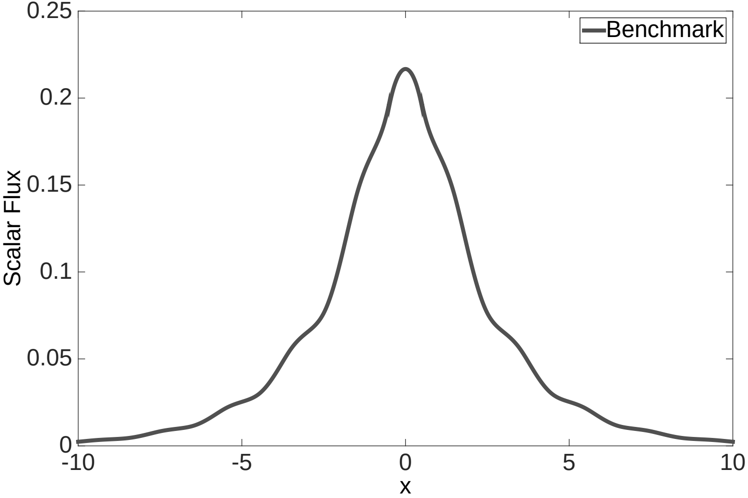
Internal source problem*



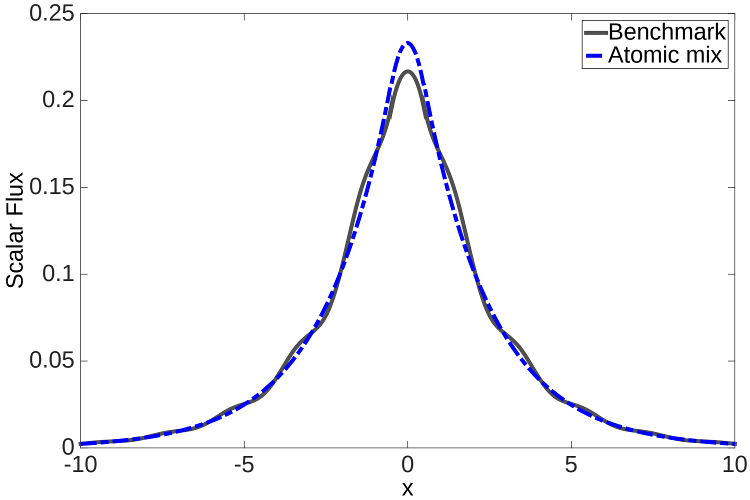
- Rod geometry transport
- Isotropic scattering
- Vacuum boundaries
- $\Sigma_{t1} = 1.0$
- scattering ratio $c = 0.95, 0.9, 0.8, 0.7, ..., 0.1, 0.0$
- Isotropic source $Q_1 = 1.0 \qquad \text{if} -0.5 \leq x \leq 0.5$

*Nuclear Science & Engineering 185, 2017

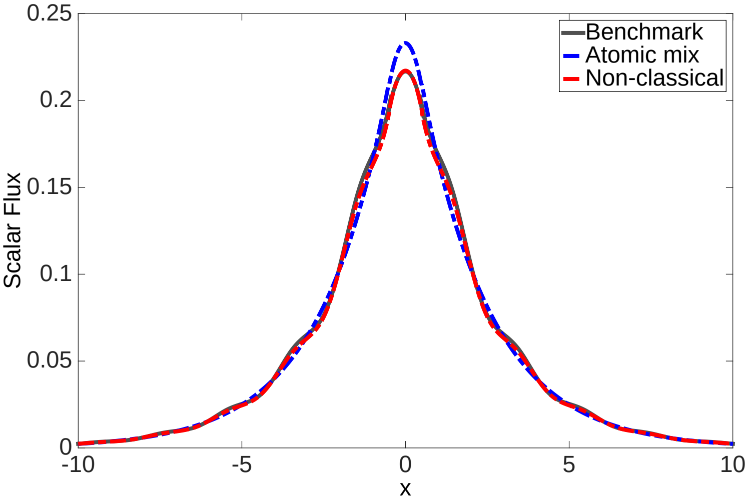
$\ell_1 = \ell_2 = 1.0$, $c = 0.1$



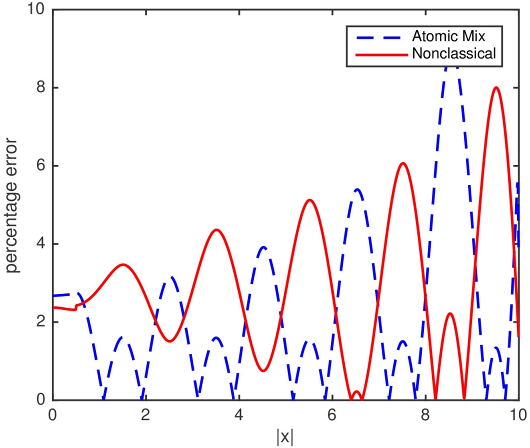
$\ell_1 = \ell_2 = 1.0, \; c = 0.1$



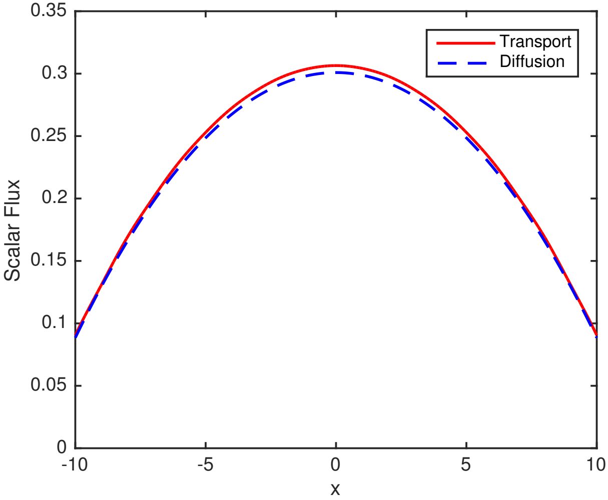
$\ell_1 = \ell_2 = 1.0, \ c = 0.1$



Relative errors ($c = 0.95, 0.9, 0.8, ..., 0.1, 0.0$)

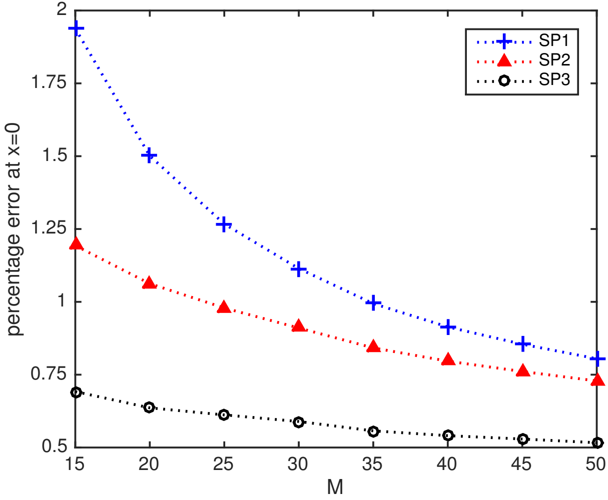


Nonclassical transport .vs. nonclassical diffusion*



*Transactions of the American Nuclear Society 114, 2016

Nonclassical SP$_N$ Error



Methods and tools

Monte Carlo

- Random numbers to sample physics
- Continuous quantities
- Statistics govern the precision
- Can have very long times

Deterministic

- Transport equation is discretized
- Physics is discretized
- Runtimes typically short
- Bad with streaming (ray effects)

Hybrid

- Deterministic adjoint solution
- Generate importance values
- Variance reduction: set weights
- Overall, time and accuracy win

Need $\Sigma_t(s)$ or $p(s)$!!!

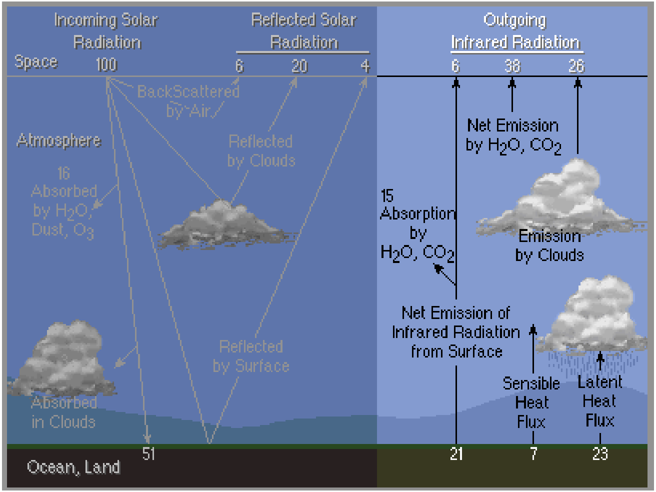
Synergies: CGI and Atmosphere

*Images by Eugene d'Eon

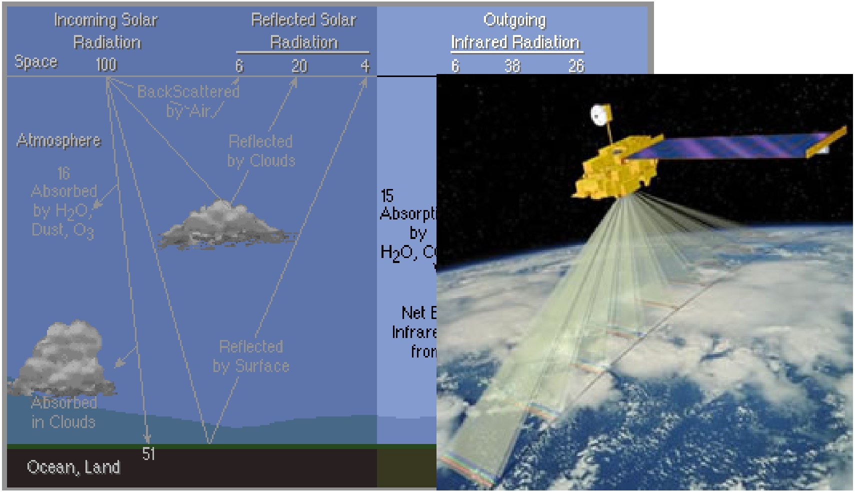
Synergies: CGI and Atmosphere

*Images from Pixar's "The Good Dinosaur"

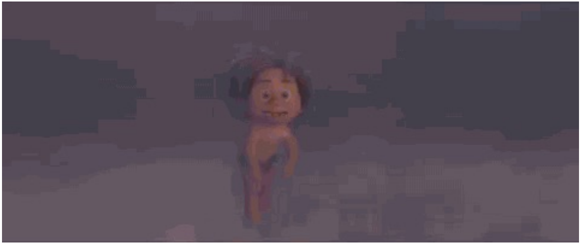
Synergies: CGI and Atmosphere



Synergies: CGI and Atmosphere

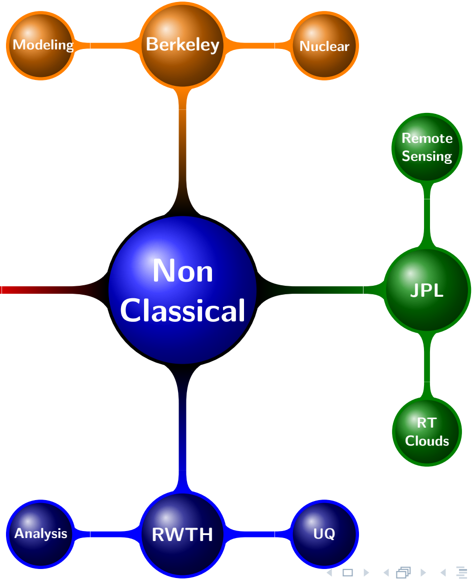


Synergies: CGI and Atmosphere

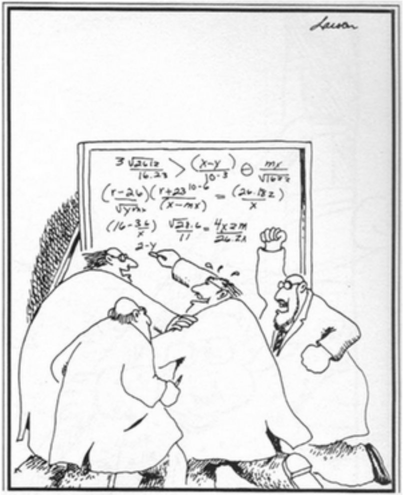


*Images from Pixar's "The Good Dinosaur"

The future... and beyond!



The future... and beyond!



"Go for it, Sidney! You've got it! You've got it! Good hands! Don't choke!"

Thank you for your attention!!!

Where to find me:

- Website:
  ricvasques.github.io
- GitHub:
  github.com/ricvasques
- Twitter:
  @Nuclear_mat
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  rvasques@berkeley.edu

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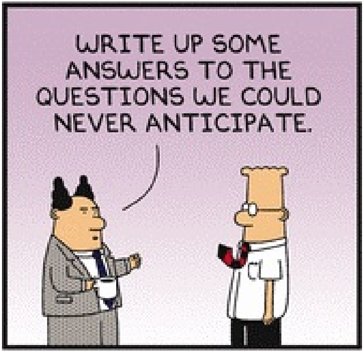
Questions?



BACKUP

Brief History

It all started in the early 2000's with the atmospheric community investigating "nonclassical" attenuation of photons in clouds. After that:

2006 Discussion on "nonclassical" photon transport in atmospheric clouds (cf. Davis; *Granlibakken Conference*)

2007 Larsen; M&C (Monterey)

2009 Vasques & Larsen; *M&C (Saratoga Springs)*

2010 Frank & Goudon; *Kinetic and Related Models*

2011 Larsen & Vasques; *Journal of Quant. Spectroscopy & Radiative Transfer*

2011 Marklof & Strömbergsson; *Annals of Mathematics*

2012 Golse; *Nonlinear Partial Differential Equations*

2013 Vasques; *M&C (Sun Valley)*

2013 Krycki, Berthon, Frank, Turpault; *Math, Methods in the Applied Sciences*

2013 d'Eon; *Transport Theory and Statistical Physics*

Brief History

2014 Vasques & Larsen; *Annals of Nuclear Energy (2 papers)*

2015 Frank, Kricky, Larsen, Vasques; *SIAM Journal on Applied Mathematics*

2015 Vasques & Kricky; *M&C (Nashville)*

2015 Vasques & Kricky; *ICTT (Taormina)*

2016 Vasques; *Applied Mathematics Letters*

2016 Vasques, Slaybaugh, Krycki; *Transactions ANS*

2017 Vasques, Krycki, Slaybaugh; *Nuclear Science and Engineering*

2017 Vasques, Slaybaugh; *M&C (South Korea)*

2017 Vasques, Segatto, Slaybaugh; *in preparation*

The nonclassical linear Boltzmann equation

Consider the infinite-medium steady-state purely-absorbing transport problem:

$$\boxed{\boldsymbol{\Omega} \cdot \nabla \Psi(\boldsymbol{x}, \boldsymbol{\Omega}) + \Sigma_t \Psi(\boldsymbol{x}, \boldsymbol{\Omega}) = \frac{Q(\boldsymbol{x})}{4\pi} \, .} \tag{1}$$

The solution of the related time-dependent problem

$$\frac{1}{v}\frac{\partial f}{\partial t}(\boldsymbol{x}, \boldsymbol{\Omega}, t) + \boldsymbol{\Omega} \cdot \nabla f(\boldsymbol{x}, \boldsymbol{\Omega}, t) + \Sigma_t f(\boldsymbol{x}, \boldsymbol{\Omega}, t) = 0 \, , \tag{2a}$$

$$f(\boldsymbol{x}, \boldsymbol{\Omega}, 0^+) = \frac{Q(\boldsymbol{x})}{4\pi} \, , \tag{2b}$$

satisfies:

$$\int_0^\infty f(\boldsymbol{x}, \boldsymbol{\Omega}, t)\, dt = \Psi(\boldsymbol{x}, \boldsymbol{\Omega}) \, . \tag{3}$$

Eqs. (2) can be written more compactly as:

$$\boxed{\frac{1}{v}\frac{\partial f}{\partial t}(\boldsymbol{x}, \boldsymbol{\Omega}, t) + \boldsymbol{\Omega} \cdot \nabla f(\boldsymbol{x}, \boldsymbol{\Omega}, t) + \Sigma_t f(\boldsymbol{x}, \boldsymbol{\Omega}, t) = \delta(t)\frac{Q(\boldsymbol{x})}{4\pi} \, .} \tag{4}$$

To proceed, we convert Eq. (4) from t = time to $s = vt$ = path-length.

The nonclassical linear Boltzmann equation

We let $\Sigma_t = \Sigma_t(s)$ to obtain the equation for a purely-absorbing system:

$$\boxed{\frac{\partial}{\partial s}\psi(\boldsymbol{x}, \boldsymbol{\Omega}, s) + \boldsymbol{\Omega} \cdot \boldsymbol{\nabla}\psi(\boldsymbol{x}, \boldsymbol{\Omega}, s) + \Sigma_t(s)\psi(\boldsymbol{x}, \boldsymbol{\Omega}, s) = \delta(s)\frac{Q(\boldsymbol{x})}{4\pi}\ .} \tag{5}$$

The classical angular flux $\Psi(\boldsymbol{x}, \boldsymbol{\Omega})$ is defined in terms of $\psi(\boldsymbol{x}, \boldsymbol{\Omega}, s)$ by:

$$\Psi(\boldsymbol{x}, \boldsymbol{\Omega}) = \int_0^\infty \psi(\boldsymbol{x}, \boldsymbol{\Omega}, s)\, ds\ . \tag{6}$$

To include scattering in Eq. (5), we note that:

$$\left[\int_0^\infty \Sigma_t(s')\psi(\boldsymbol{x}, \boldsymbol{\Omega}', s')\, ds'\right] dVd\Omega' = \textbf{ rate at which particles in } dVd\Omega' \textbf{ about } (\boldsymbol{x}, \boldsymbol{\Omega}') \textbf{ experience collisions.} \tag{7}$$

Multiplying by $\frac{c}{4\pi} d\Omega$, we get:

$$\frac{c}{4\pi}\left[\int_0^\infty \Sigma_t(s')\psi(\boldsymbol{x}, \boldsymbol{\Omega}', s')\, ds'\right] dVd\Omega' d\Omega = \textbf{ rate at which particles in } dVd\Omega' \textbf{ about } (\boldsymbol{x}, \boldsymbol{\Omega}') \textbf{ scatter into } d\Omega \textbf{ about } \Omega\ . \tag{8}$$

The nonclassical linear Boltzmann equation

Integrating Eq. (8) over $\boldsymbol{\Omega}'$, we get:

$$\left[\frac{c}{4\pi}\int_{4\pi}\int_0^\infty \Sigma_t(s')\psi(\boldsymbol{x},\boldsymbol{\Omega}',s')\,ds'd\Omega'\right] dVd\Omega = \textbf{ rate at which}$$

particles in dV about $\boldsymbol{x}$ scatter into $d\Omega$ about Ω.

Multiplying this result by $\delta(s)ds$, we obtain:

$$\left[\delta(s)\frac{c}{4\pi}\int_{4\pi}\int_0^\infty \Sigma_t(s')\psi(\boldsymbol{x},\boldsymbol{\Omega}',s')\,ds'd\Omega'\right] dVd\Omega ds = \textbf{ rate at}$$

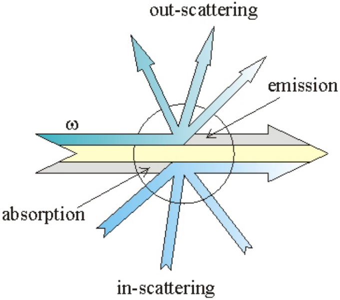
which particles inscatter into $dVd\Omega\,ds$ about $(\boldsymbol{x},\Omega,s)$. (9)

Finally, we add the bracketed term in Eq. (9) to the right side of Eq. (5) and obtain the Non-Classical Boltzmann Equation

$$\frac{\partial\psi}{\partial s}(\boldsymbol{x},\boldsymbol{\Omega},s) + \boldsymbol{\Omega}\cdot\boldsymbol{\nabla}\psi(\boldsymbol{x},\boldsymbol{\Omega},s) + \Sigma_t(s)\psi(\boldsymbol{x},\boldsymbol{\Omega},s)$$
$$= \delta(s)\frac{c}{4\pi}\int_{4\pi}\int_0^\infty \Sigma_t(s')\psi(\boldsymbol{x},\boldsymbol{\Omega}',s')\,ds'd\Omega' + \delta(s)\frac{Q(\boldsymbol{x})}{4\pi}\,. \qquad (10)$$

Balance equation

Rate of Change = Gain − Loss



Gain

- Source (emission)
- In-scattering *

Loss

- Net leakage
- Absorption
- Out-scattering *

Integral equation formulation

Integro-differential equation

$$\frac{\partial\psi}{\partial s}(\boldsymbol{x},\boldsymbol{\Omega},s) + \boldsymbol{\Omega}\cdot\boldsymbol{\nabla}\psi(\boldsymbol{x},\boldsymbol{\Omega},s) + \Sigma_t(\boldsymbol{\Omega},s)\psi(\boldsymbol{x},\boldsymbol{\Omega},s)$$
$$= \frac{\delta(s)}{4\pi}\left[c\int_{4\pi}\int_0^\infty \Sigma_t(\boldsymbol{\Omega}',s')\psi(\boldsymbol{x},\boldsymbol{\Omega}',s')\,ds'd\Omega' + Q(\boldsymbol{x})\right]$$

Integral equation

$$f(\boldsymbol{x}) = \int\int\int [cf(\boldsymbol{x}') + Q(\boldsymbol{x}')]\frac{p(|\boldsymbol{x}'-\boldsymbol{x}|)}{4\pi|\boldsymbol{x}'-\boldsymbol{x}|^2}dV'$$

where

$$f(\boldsymbol{x}) = \int_0^\infty\int_{4\pi}\Sigma_t(s)\psi(\boldsymbol{x},\boldsymbol{\Omega},s)d\Omega ds = \text{collision-rate density}$$

Integral representation of classical models

We can use the integral formulation to find representations of classical models. All we need to do is find the correct $p(s)$.

If $p(s) = \Sigma_t e^{-\Sigma_t s}$, we obtain **classical transport**.

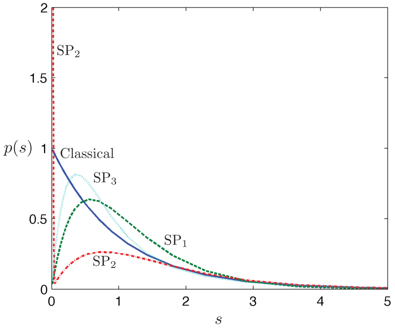
If $p(s) = 3\Sigma_t^2 s e^{-\sqrt{3}\Sigma_t s}$, we obtain **classical diffusion**:

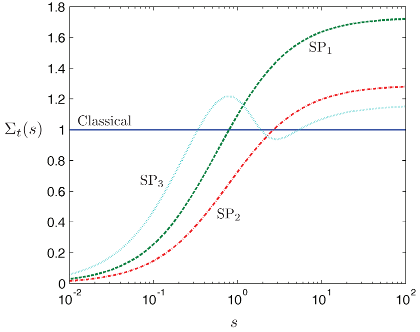
$$-\frac{1}{3\Sigma_t}\nabla^2\phi(\boldsymbol{x}) + (1-c)\Sigma_t\phi(\boldsymbol{x}) = Q(\boldsymbol{x}).$$

This can be extended to the simplified spherical harmonics (SP_N) equations.

Diffusion-based models

This approach allows us to represent important diffusion processes as actual *transport* models:





Nonclassical diffusion as an asymptotic limit

With $\varepsilon \ll 1$, we scale:

- $\Sigma_t = O(\varepsilon^{-1})$
- $1 - c = O(\varepsilon^2)$
- $Q = O(\varepsilon)$
- $P^*(\mu_0)$ is independent of ε
- $\partial\psi/\partial s = O(\varepsilon^{-1})$

The scaled nonclassical equation becomes:

$$\frac{1}{\varepsilon}\frac{\partial\psi}{\partial s}(\boldsymbol{x},\boldsymbol{\Omega},s) + \boldsymbol{\Omega}\cdot\boldsymbol{\nabla}\psi(\boldsymbol{x},\boldsymbol{\Omega},s) + \frac{\Sigma_t(\boldsymbol{\Omega},s)}{\varepsilon}\psi(\boldsymbol{x},\boldsymbol{\Omega},s)$$
$$= \delta(s)\int_{4\pi}\int_0^\infty \left[P^*(\boldsymbol{\Omega}\cdot\boldsymbol{\Omega}') - \varepsilon^2\frac{1-c}{4\pi}\right]\frac{\Sigma_t(\boldsymbol{\Omega}',s')}{\varepsilon}\psi(\boldsymbol{x},\boldsymbol{\Omega}',s')\,ds'\,d\Omega'$$
$$+\,\varepsilon\delta(s)\frac{Q(\boldsymbol{x})}{4\pi}\,.$$

We seek a solution of this equation of the form:

$$\psi(\boldsymbol{x},\boldsymbol{\Omega},s) = \sum_{n=0}^{\infty}\varepsilon^n\psi^{(n)}(\boldsymbol{x},\boldsymbol{\Omega},s)\,.$$

Nonclassical diffusion as an asymptotic limit

This solution is found to be*

$$\psi(\boldsymbol{x}, \boldsymbol{\Omega}, s) = \frac{\Phi^{(0)}(\boldsymbol{x})}{4\pi} \frac{e^{-\int_0^s \Sigma_t(\boldsymbol{\Omega}, s')ds'}}{\langle s \rangle} + O(\varepsilon) \, ,$$

where $\langle s^n \rangle$ is the nth moment of $p(\boldsymbol{\Omega}, s)$, and $\Phi^{(0)}(\boldsymbol{x})$ satisfies the nonclassical diffusion equation

$$-\left[\mathrm{D}_{xx}\frac{\partial^2}{\partial x^2} + \mathrm{D}_{yy}\frac{\partial^2}{\partial y^2} + \mathrm{D}_{zz}\frac{\partial^2}{\partial z^2} + \mathrm{D}_{xy}\frac{\partial^2}{\partial x \partial y} + \mathrm{D}_{xz}\frac{\partial^2}{\partial x \partial z} + \mathrm{D}_{yz}\frac{\partial^2}{\partial y \partial z}\right]\Phi^{(0)}(\boldsymbol{x}) + \frac{1-c}{\langle s \rangle}\Phi^{(0)}(\boldsymbol{x}) = Q(\boldsymbol{x}) \, ,$$

* *Annals of Nuclear Energy (2014)*

The nonclassical diffusion tensor

The general case has diffusion coefficients given by

$$\mathrm{D}_{uu} = \frac{1}{4\pi\langle s\rangle}\int_{4\pi}\left(\frac{\langle s_{\boldsymbol{\Omega}}^2\rangle(\boldsymbol{\Omega})}{2}\Omega_u - \langle s_{\boldsymbol{\Omega}}\rangle(\boldsymbol{\Omega})\tau_u(\boldsymbol{\Omega})\right)\Omega_u d\Omega,$$

$$\mathrm{D}_{uv} = \frac{1}{4\pi\langle s\rangle}\int_{4\pi}\left(\langle s_{\boldsymbol{\Omega}}^2\rangle(\boldsymbol{\Omega})\Omega_u\Omega_v - \langle s_{\boldsymbol{\Omega}}\rangle(\boldsymbol{\Omega})[\tau_u(\boldsymbol{\Omega})\Omega_v + \tau_v(\boldsymbol{\Omega})\Omega_u]\right) d\Omega,$$

where $\boldsymbol{\tau}(\boldsymbol{\Omega})$ satisfies the Fredholm integral equation of the second kind

$$\boldsymbol{\tau}(\boldsymbol{\Omega}) = \int_{4\pi} P^*(\boldsymbol{\Omega}\cdot\boldsymbol{\Omega}')\boldsymbol{\tau}(\boldsymbol{\Omega}')d\Omega' - \int_{4\pi}\boldsymbol{\Omega}' P^*(\boldsymbol{\Omega}\cdot\boldsymbol{\Omega}')\langle s_{\boldsymbol{\Omega}}\rangle(\boldsymbol{\Omega}')d\Omega'$$

- If scattering is isotropic, $\boldsymbol{\tau}(\boldsymbol{\Omega}) = 0$ and

$$\mathrm{D}_{uu} = \frac{1}{2\langle s\rangle}\left(\frac{1}{4\pi}\int_{4\pi}\langle s_{\boldsymbol{\Omega}}^2\rangle(\boldsymbol{\Omega})\Omega_u^2 d\Omega\right), \qquad \mathrm{D}_{uv} = \frac{1}{\langle s\rangle}\left(\frac{1}{4\pi}\int_{4\pi}\langle s_{\boldsymbol{\Omega}}^2\rangle(\boldsymbol{\Omega})\Omega_u\Omega_v d\Omega\right)$$

The nonclassical diffusion tensor

♦ If scattering is isotropic and there is azimuthal symmetry

$$\mathrm{D}_{uu} = \frac{1}{2\langle s\rangle}\left[\frac{1}{4\pi}\int_{-1}^{1}\langle s_{\Omega}^2\rangle(\mu)\left(\int_{-\pi}^{\pi}\Omega_u^2 d\varphi\right)d\mu\right], \qquad \mathrm{D}_{uv} = 0$$

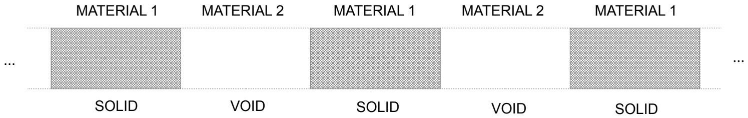
♦ If $\Sigma_t = \Sigma_t(s)$ is independent of direction $\boldsymbol{\Omega}$,

$$\mathrm{D} = \mathrm{D}_{uu} = \frac{1}{3}\left(\frac{\langle s^2\rangle}{2\langle s\rangle} + \frac{c\overline{\mu}_0}{1 - c\overline{\mu}_0}\langle s\rangle\right), \qquad \mathrm{D}_{uv} = 0$$

♦If Σ_t is constant, then the generalized theory reduces to the classic theory

$$\mathrm{D} = \mathrm{D}_{uu} = [3\Sigma_t(1 - c\overline{\mu}_0)]^{-1}$$

1-D diffusive system



- Rod geometry transport
- Isotropic scattering
- Vacuum boundaries
- Isotropic source
- We define $M = \varepsilon^{-1}$, and
  - $\ell_1 = \ell_2 = 1 \Longrightarrow \ell = 2$
  - $-M \leq x \leq M \Longrightarrow \ell M = O(\varepsilon^{-1})$
  - $\Sigma_{t1} = 1 = O(1)$
  - $1 - c = M^{-2} = O(\varepsilon^2)$
  - $Q_1 = 2M^{-2} = O(\varepsilon^2)$

1-D nonclassical equations

Nonclassical transport

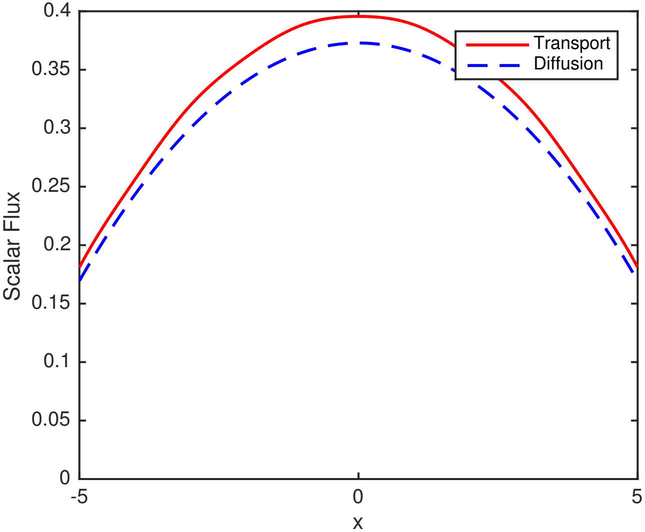
$$\frac{\partial \psi^{\pm}}{\partial s}(x,s) \pm \frac{\partial \psi^{\pm}}{\partial x}(x,s) + \Sigma_t(s)\psi^{\pm}(x,s)$$
$$= \frac{\delta(s)}{2}\left[c\int_0^\infty \Sigma_t(s')\left[\psi^{\pm}(x,s') + \psi^{\mp}(x,s')\right]ds' + Q(x)\right],$$

$$\phi(x) = \frac{1}{2}\int_0^\infty \left[\psi^{\pm}(x,s) + \psi^{\mp}(x,s)\right]ds$$

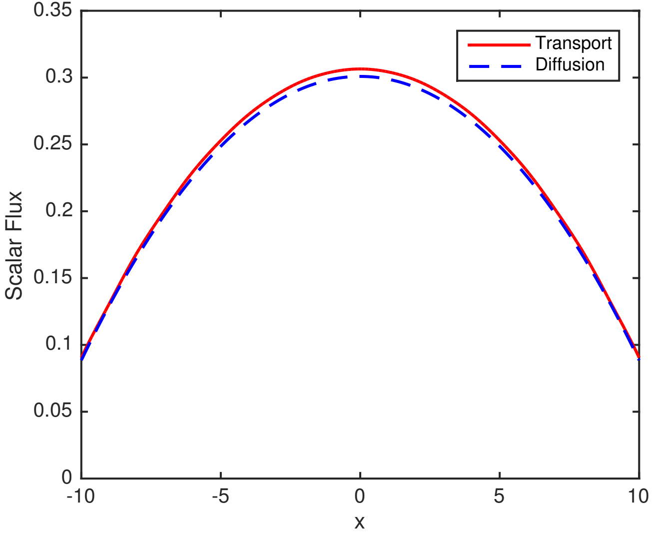
Nonclassical diffusion

$$-\frac{\langle s^2\rangle}{2\langle s\rangle}\frac{d^2\hat{\phi}_0}{dx^2}(x) + \frac{1-c}{\langle s\rangle}\hat{\phi}_0(x) = Q(x)$$

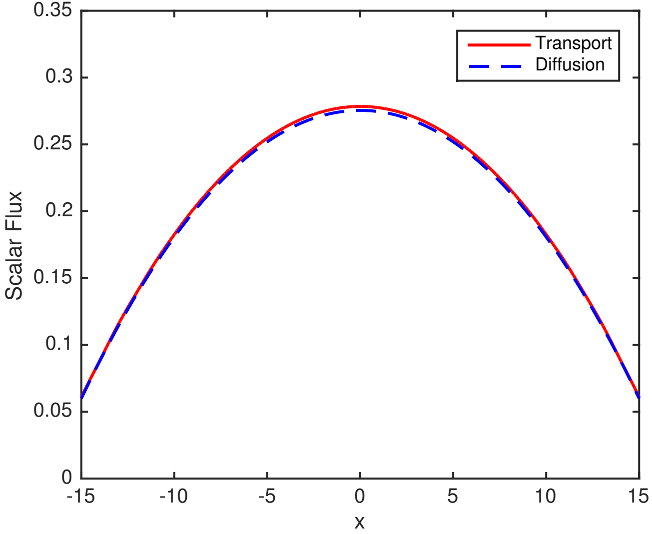
Numerical results: $M = 5$



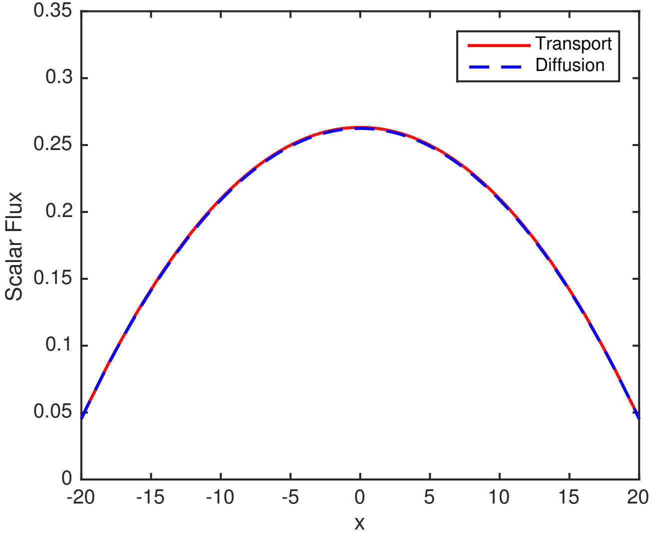
Numerical results: $M = 10$



Numerical results: $M = 15$



Numerical results: $M = 20$



Important Questions

- Does the non-classical approach yield better accuracy than Atomic Mix?
- Given the potentially long streaming paths between pebbles, is a diffusion description sufficiently accurate?

YES!!

- The non-classical theory outperforms the Atomic Mix approach and its corrections for 2-D and 3-D model PBRs with random and crystal structures
- The non-classical theory yields accurate estimates of the diffusion coefficients, while the estimates obtained with the classical methods are very sensitive to changes in the core dimensions

The Non-Classical Diffusion Equation

In the case of **isotropic scattering** and **azimuthal symmetry**, the *Non-Classical Diffusion Equation* is

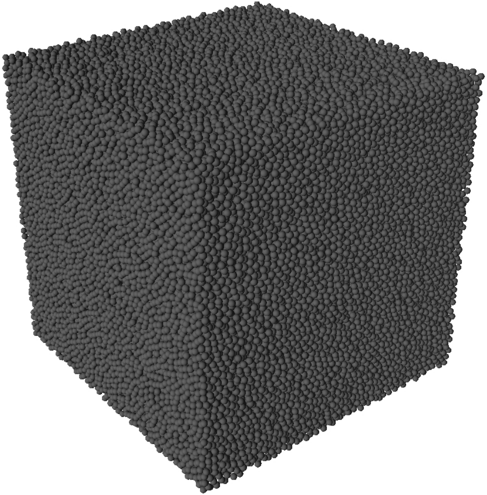
$$-\mathrm{D}_x \frac{\partial^2}{\partial x^2}\Phi(\boldsymbol{x}) - \mathrm{D}_y \frac{\partial^2}{\partial y^2}\Phi(\boldsymbol{x}) - \mathrm{D}_z \frac{\partial^2}{\partial z^2}\Phi(\boldsymbol{x}) + \frac{1-c}{\langle s \rangle}\Phi(\boldsymbol{x}) = Q(\boldsymbol{x}), \tag{11a}$$

$$\mathrm{D}_u = \frac{1}{2\langle s \rangle}\frac{1}{4\pi}\int_{4\pi} s^2_{\boldsymbol{\Omega}}(\boldsymbol{\Omega})\Omega_u^2 d\Omega, \tag{11b}$$

where $s^2_{\boldsymbol{\Omega}}(\boldsymbol{\Omega})$ is the mean-squared free path of a neutron in the direction $\boldsymbol{\Omega}$.

We see from Eq. (11b) that the diffusion coefficients given by the Non-Classical theory can differ in different directions.

Model Pebble Bed System



Parameters of Fuel Pebbles

Table 1: Parametes for fuel pebbles with diameter d

Problem	dΣ_t	dΣ_s	dΣ_a	$c = \Sigma_s/\Sigma_t$	$P(\mathbf{\Omega} \cdot \mathbf{\Omega}')$
1	1.0	0.99	0.01	0.99	$1/4\pi$
2	2.0	0.995	0.005	0.9975	$1/4\pi$

Results

Table 7: Diffusion coefficients in random structures

Problem		Monte Carlo		Atomic Mix and Corrections			"Old" GLBE	New GLBE	
		D_x^{mc}	D_z^{mc}	D^{am}	D^B	D^L	D^{iso}	D_x^{gt}	D_z^{gt}
1	Diffusion Coeff.	0.6144	0.6157	0.5617	0.6009	0.5990	0.6147	0.6146	0.6150
	error_x (%)	-	-	8.580	2.201	2.506	0.049	0.029	-
	error_z (%)	-	-	8.776	2.411	2.716	0.166	-	0.126
2	Diffusion Coeff.	0.3286	0.3295	0.2809	0.3200	0.3214	0.3326	0.3324	0.3329
	error_x (%)	-	-	14.542	2.617	2.214	1.204	1.154	-
	error_z (%)	-	-	14.771	2.877	2.475	0.934	-	1.034

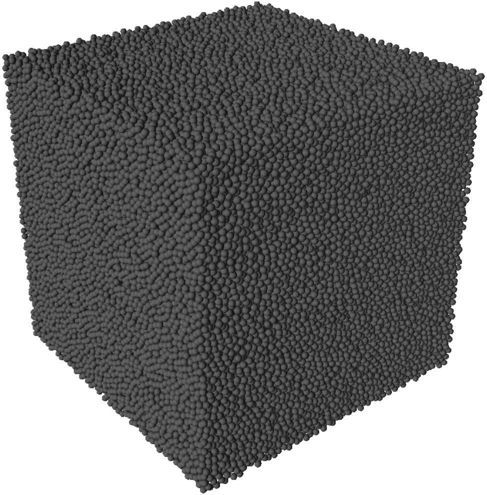
Important Questions

- Does the random piling of pebbles through gravity significantly affect the diffusion of particles in an anisotropic way?

YES and NO

- Anisotropy away from the boundaries is neglectable, but there is strong indication of a boundary region in which neutrons travel significantly further along the walls

Model Pebble Bed System



Boundary Effect

Parameters for Fuel Pebbles with Diameter d

Problem	$d\Sigma_{t,1}$	$d\Sigma_{s,1}$	$d\Sigma_{a,1}$	$c = \Sigma_{s,1}/\Sigma_{t,1}$	$P(\mathbf{\Omega} \cdot \mathbf{\Omega})$
1	1.0	0.99	0.01	0.99	$1/4\pi$
2	2.0	1.995	0.005	0.9975	$1/4\pi$
3	4.0	3.9975	0.0025	0.999375	$1/4\pi$

Results

Ensemble-Averaged Monte Carlo Transport

Problem	$\langle s \rangle / d$	$\langle s^2 \rangle / d^2$	$\langle x^2 \rangle / d^2$	$\langle y^2 \rangle / d^2$	$\langle \rho^2 \rangle / d^2$
1	1.7271	6.4795	210.8987	216.7292	644.3571
2	0.8634	1.7611	225.9157	232.6521	691.2200
3	0.4316	0.5184	255.8249	264.6351	785.0952

Relative statistical error (%) with 95% confidence

Problem	$\langle s \rangle / d$	$\langle s^2 \rangle / d^2$	$\langle x^2 \rangle / d^2$	$\langle y^2 \rangle / d^2$	$\langle \rho^2 \rangle / d^2$
1	0.1299	0.2848	0.2908	0.2614	0.2327
2	0.1130	0.2748	0.2549	0.2711	0.2398
3	0.0971	0.2757	0.2262	0.2260	0.2021

Problem 1

Model	$\frac{\langle x^2 \rangle^{1/2}}{d}$	Error(%)	$\frac{\langle y^2 \rangle^{1/2}}{d}$	Error(%)	$\frac{\langle \rho^2 \rangle^{1/2}}{d}$	Error(%)
Monte Carlo	14.5224	0.1454	14.7217	0.1307	25.3842	0.1164
Non-Classical	14.6439	0.8372	14.7225	0.0052	25.4548	0.2781
Atomic Mix (Γ_1)	17.3804	19.6806	17.3804	18.0598	30.1038	18.5927
Atomic Mix (Γ_2)	14.8939	2.5586	14.8939	1.1697	25.7970	1.6264
Atomic Mix (Γ_3)	14.0990	2.9154	14.0990	4.2302	24.4201	3.7979

Problem 2

Model	$\frac{\langle x^2 \rangle^{1/2}}{d}$	Error(%)	$\frac{\langle y^2 \rangle^{1/2}}{d}$	Error(%)	$\frac{\langle \rho^2 \rangle^{1/2}}{d}$	Error(%)
Monte Carlo	15.0305	0.1275	15.2529	0.1355	26.2911	0.1199
Non-Classical	15.2756	1.6309	15.3474	0.6193	26.5411	0.9510
Atomic Mix (Γ_1)	17.3804	15.6345	17.3804	13.9481	30.1038	14.5213
Atomic Mix (Γ_2)	14.8939	0.9086	14.8939	2.3537	25.7970	1.8656
Atomic Mix (Γ_3)	14.0990	6.1976	14.0990	7.5656	24.4201	7.1134

Problem 3

Model	$\frac{\left\langle x^2 \right\rangle^{1/2}}{d}$	Error(%)	$\frac{\left\langle y^2 \right\rangle^{1/2}}{d}$	Error(%)	$\frac{\left\langle \rho^2 \right\rangle^{1/2}}{d}$	Error(%)
Monte Carlo	15.9945	0.1131	16.2676	0.1130	28.0195	0.1011
Non-Classical	16.5738	3.6217	16.6539	2.3747	28.7992	2.7827
Atomic Mix (Γ_1)	17.3804	8.6649	17.3804	6.8408	30.1038	7.4529
Atomic Mix (Γ_2)	14.8939	6.8811	14.8939	8.4442	25.7970	7.9329
Atomic Mix (Γ_3)	14.0990	11.8514	14.0990	13.3310	24.4201	12.8354

The Levermore-Pomraning Equations

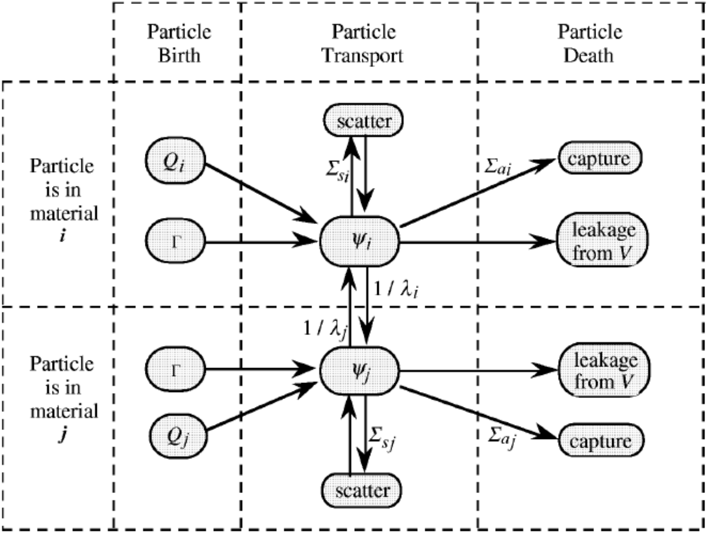
The Levermore-Pomraning (LP) equations describe the transport process in a set of coupled equations:

$$
\begin{aligned}
\frac{1}{v}\frac{[p_i \partial \psi_i]}{\partial t}(\boldsymbol{x}, \boldsymbol{\Omega}, t) &+ \\
&+ \boldsymbol{\Omega} \cdot \nabla [p_i \psi_i](\boldsymbol{x}, \boldsymbol{\Omega}, t) + \Sigma_{t,i}[p_i \psi_i](\boldsymbol{x}, \boldsymbol{\Omega}, t) = \\
&= \frac{c_i \Sigma_{t,i}}{4\pi} \int_{4\pi} [p_i \psi_i](\boldsymbol{x}, \boldsymbol{\Omega}', t) d\Omega' + \frac{p_i Q_i(\boldsymbol{x})}{4\pi} + \\
&+ \left(\frac{[p_j \psi_j]}{\lambda_j}(\boldsymbol{x}, \boldsymbol{\Omega}, t) - \frac{[p_i \psi_i]}{\lambda_i}(\boldsymbol{x}, \boldsymbol{\Omega}, t) \right)
\end{aligned}
$$

$$
\boxed{\langle \psi \rangle(\boldsymbol{x}, \boldsymbol{\Omega}, t) = p_1 \psi_1(\boldsymbol{x}, \boldsymbol{\Omega}, t) + p_2 \psi_2(\boldsymbol{x}, \boldsymbol{\Omega}, t)}
$$

A closure is needed to obtain the coupling term

The Levermore-Pomraning Process



Pros and Cons

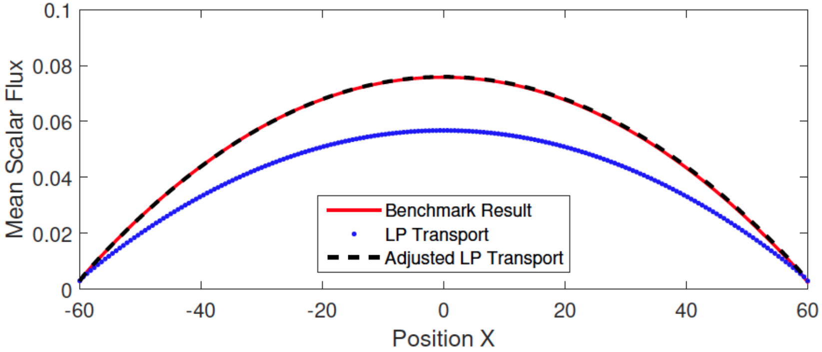
Main advantages

+ Physically appealing
+ Exact for purely absorbing Markovian mixtures
+ Decouples the ensemble-averaged flux

Main disadvantages

- Harder to implement
- Inaccurate closure when scattering takes place
- Simplifications are not straightforward

Parenthesis - Adjusted LP



1-D models

Classical Transport

$$\pm\frac{\partial\psi^\pm}{\partial x}(x) + \Sigma_t(x)\psi^\pm(x) = \frac{c\Sigma_t(x)}{2}\left[\psi^+(x) + \psi^-(x)\right] + \frac{Q(x)}{2}$$

Atomic Mix

$$\pm\frac{\partial\langle\psi^\pm\rangle}{\partial x}(x) + \langle\Sigma_t\rangle\langle\psi^\pm\rangle(x) = \frac{c\langle\Sigma_t\rangle}{2}\left[\langle\psi^+\rangle(x) + \langle\psi^-\rangle(x)\right] + \frac{\langle Q\rangle}{2},$$

$$\langle\Sigma_t\rangle = P_1\Sigma_{t1} + P_2\Sigma_{t2} \qquad \langle Q\rangle = P_1 Q_1 + P_2 Q_2$$

Nonclassical Boltzmann

$$\frac{\partial\psi^\pm}{\partial s}(x,s) \pm \frac{\partial\psi^\pm}{\partial x}(x,s) + \Sigma_t(s)\psi^\pm(x,s)$$

$$= \delta(s)\frac{c}{2}\int_0^\infty \Sigma_t(s')[\psi^+(x,s') + \psi^-(x,s')]ds' + \delta(s)\frac{\langle Q\rangle}{2}.$$

The nonclassical model

We can rewrite the nonclassical equation in the following

Initial Value Form

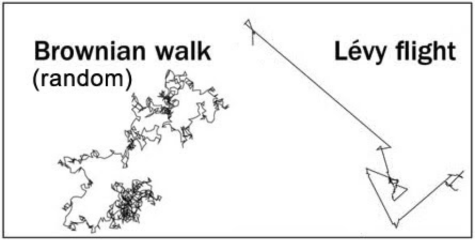
$$\frac{\partial \psi^{\pm}}{\partial s}(x,s) \pm \frac{\partial \psi^{\pm}}{\partial x}(x,s) + \Sigma_t(s)\psi^{\pm}(x,s) = 0,$$

$$\psi^{\pm}(x,0) = \frac{c}{2}\int_0^{\infty} \Sigma_t(s')[\psi^{+}(x,s') + \psi^{-}(x,s')]ds' + \frac{\langle Q \rangle}{2}.$$

- Initial value is coupled to the full solution
- Equation can be solved in a source-iteration manner: iterate between second and first equations

Lévy flights

A Lévy flight is a random walk in which the step-lengths have a probability distribution that is heavy-tailed:



Applications:

- Earthquake data analysis
- Financial mathematics
- Cryptography
- Foraging hypothesis

The nonclassical model

We adapt a finite volume HLL scheme for the nonclassical equation:

Discretized Equation

$$\frac{\psi_m^{n+1,\pm} - \psi_m^{n,\pm}}{\Delta s} \pm \frac{\psi_{m+1}^{n,\pm} - \psi_{m-1}^{n,\pm}}{2\Delta x} - \frac{\psi_{m+1}^{n,\pm} - 2\psi_m^{n,\pm} + \psi_{m-1}^{n,\pm}}{2\Delta x} + \Sigma_t^n \psi_m^{n,\pm} = 0,$$

$$\psi_m^{0,\pm} = \frac{c}{2}\sum_{n=0}^{\infty} \omega_n \Sigma_t^n \left(\psi_m^{n,+} + \psi_m^{n,-}\right) + \frac{Q_m}{2}.$$

- Second central difference term is numerical diffusion.
- Contraction rate of source-iteration is c.
- $\Delta x = 2^{-7}$, CFL $= 0.5$.
- Numerical integration by trapezoidal rule, with weights given by ω_n.
- Numerical integration is cut off at $s_{\max} = 80$.

P_N Equations

Consider the planar (slab) geometry P_N equations: for $l' = 0, 1, \ldots,$ we have

$$\left(\frac{l'+1}{2l'+1}\right)\frac{d}{dx}\phi_{l'+1}(x) + \left(\frac{l'}{2l'+1}\right)\frac{d}{dx}\phi_{l'-1}(x) + \Sigma_t(x)\phi_{l'} = \Sigma_{sl'}(x)\phi_{l'}(x) + s_{l'}(x)\,,$$

with

$$\phi_{-1} = 0 \quad \text{and} \quad \phi_{N+1} = 0 \quad \left(\text{or} \quad \frac{d}{dx}\phi_{N+1} = 0\right).$$

The classical simplified P_N equations (SP_N) can be obtained from the equation above in a heuristic way.

"Heuristic" Derivation of SP_N Equations

First, for odd values of l', $\phi_{l'}$ is replaced by a vector:

$$\phi_{l'} \rightarrow \vec{\phi}_{l'} = (\phi_{l'}^{x}, \phi_{l'}^{y}, \phi_{l'}^{z})^t \,.$$

Then, in the even l' equations the derivative in x is replaced by a divergence:

$$\frac{d}{dx} \rightarrow \nabla \cdot \,;$$

and in the odd l' equations the x derivative is changed to a gradient:

$$\frac{d}{dx} \rightarrow \nabla$$

"Heuristic" Derivation of SP$_N$ Equations

This allows us to write the first-order form of the SP$_N$ equations as

$$\nabla \cdot \vec{\phi}_1 + \Sigma_a \phi_0 = s_0 \,,$$

$$\left(\frac{l'+1}{2l'+1}\right) \nabla \phi_{l'+1} + \left(\frac{l'}{2l'+1}\right) \nabla \phi_{l'-1} + \Sigma_t \vec{\phi}_{l'} = \Sigma_{sl'} \vec{\phi}_{l'} + s_{l'} \,, \text{for odd } l',$$

$$\left(\frac{l'+1}{2l'+1}\right) \nabla \cdot \vec{\phi}_{l'+1} + \left(\frac{l'}{2l'+1}\right) \nabla \cdot \vec{\phi}_{l'-1} + \Sigma_t \phi_{l'} = \Sigma_{sl'} \phi_{l'} + s_{l'} \,, \text{for even } l' > 0.$$

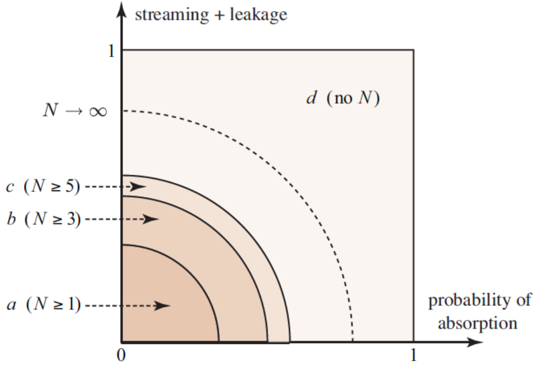
We can get rid of the odd moments and rewrite them in their second-order form by using the relation

$$\vec{\phi}_{l'} = -\frac{1}{\Sigma_t - \Sigma_{sl'}} \left(\frac{l'}{2l'+1} \nabla \phi_{l'-1} + \frac{l'+1}{2l'+1} \nabla \phi_{l'+1}\right) .$$

Why SP_N?

1. Mathematical structure is simpler: SP_N are elliptic; P_N are hyperbolic
2. The SP_N equations can be understood as a "super" diffusion theory
3. The structure of the SP_N equations is that of a coupled system of diffusion equations
4. Much simpler than P_N in multidimensional problems (with fewer equations)
5. Simpler code implementation: just use/adapt a diffusion code!!
6. The SP_N equations contain more "transport physics" than the diffusion equations.

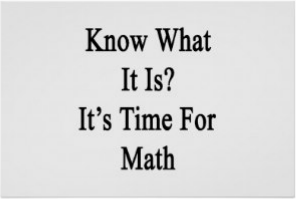
Qualitative Behavior of SP$_N$ Equations



The amounts of absorption and streaming/leakage are indicated on arbitrary scales ranging from 0 to 1.

A Thought...

- Nonclassical transport requires one to know $\Sigma_t(s)$ (or $p(s)$), which is not easy to obtain
- Nonclassical *diffusion* is simpler: it only requires the first and second moments of $p(s)$ to be known
- Can we extend this result to obtain more accurate diffusion approximations? Maybe using something similar to the SP_N approach?



Asymptotic Analysis

Let us write the nonclassical Boltzmann equation in the mathematically equivalent form

$$\frac{\partial \Psi}{\partial s}(s) + \boldsymbol{\Omega} \cdot \nabla \Psi(s) + \Sigma_t(s)\Psi(s) = 0, \qquad s > 0,$$

$$\Psi(0) = \frac{1}{4\pi}\left[\int_{4\pi}\int_0^\infty c\Sigma_t(s')\Psi(\boldsymbol{x}, \boldsymbol{\Omega}', s')ds'd\Omega' + Q(\boldsymbol{x})\right].$$

Defining $0 < \varepsilon \ll 1$, we perform the following scaling:

$$\Sigma_t(s) = \varepsilon^{-1}\Sigma_t(s/\varepsilon)$$

$$c = 1 - \varepsilon^2\kappa$$

$$Q(\boldsymbol{x}) = \varepsilon q(\boldsymbol{x})$$

where κ and q are $O(1)$.

Under this scaling,

$$\left\langle s^m \right\rangle = \varepsilon^m \int_0^\infty s^m \Sigma_t(s) e^{-\int_0^s \Sigma_t(s')ds'} ds = \varepsilon^m \left\langle s^m \right\rangle_\varepsilon,$$

where $\left\langle s^m \right\rangle_\varepsilon$ is $O(1)$.

Asymptotic Analysis

Next, we define

$$\psi(\boldsymbol{x},\boldsymbol{\Omega},s) \equiv \frac{\varepsilon\langle s\rangle_\epsilon}{e^{-\int_0^s \Sigma_t(s')ds'}}\Psi(\boldsymbol{x},\boldsymbol{\Omega},\varepsilon s).$$

This satisfies

$$\frac{\partial\psi}{\partial s}(s) + \varepsilon\boldsymbol{\Omega}\cdot\nabla\psi(s) = 0, \qquad s > 0,$$
$$\psi(0) = \frac{1}{4\pi}\left[\int_{4\pi}\int_0^\infty (1-\varepsilon^2\kappa)p(s')\psi(\boldsymbol{x},\boldsymbol{\Omega}',s')ds'd\Omega' + \varepsilon^2\langle s\rangle_\epsilon q(\boldsymbol{x})\right],$$

and the classical scalar flux can be written as

$$\Phi(\boldsymbol{x}) = \int_{4\pi}\int_0^\infty \psi(\boldsymbol{x},\boldsymbol{\Omega},s)\frac{e^{-\int_0^s \Sigma_t(s')ds'}}{\langle s\rangle_\epsilon}dsd\Omega.$$

We now integrate the first equation over $0 < s' < s$.

Asymptotic Analysis

Using the "initial condition" in s, we obtain

$$\left(I + \varepsilon\mathbf{\Omega}\cdot\nabla\int_0^s(\cdot)ds\right)\psi = \frac{1}{4\pi}\left[\int_0^\infty(1-\varepsilon^2\kappa)p(s')\varphi(\boldsymbol{x},s')ds' + \varepsilon^2\langle s\rangle_\epsilon q\right],$$

where

$$\varphi(\boldsymbol{x},s) = \int_{4\pi}\psi(\boldsymbol{x},\mathbf{\Omega},s)d\Omega.$$

Inverting the operator on the left-hand side of the above equation and expanding it in a power series, we obtain

$$\psi = \left(\sum_{n=0}^{\infty}(-\varepsilon)^n\left(\mathbf{\Omega}\cdot\nabla\int_0^s(\cdot)ds\right)^n\right)\times \left[\int_0^\infty\frac{1-\varepsilon^2\kappa}{4\pi}p(s')\varphi(\boldsymbol{x},s')ds' + \varepsilon^2\langle s\rangle_\epsilon\frac{q}{4\pi}\right].$$

Asymptotic Analysis

Next we will need the identity

$$\frac{1}{4\pi}\int_{4\pi}\left(\boldsymbol{\Omega}\cdot\nabla\int_0^s(\cdot)ds\right)^n d\Omega = \frac{1+(-1)^n}{2}\frac{3^{n/2}}{n+1}\mathcal{B}^{n/2},$$

for $n = 0, 1, 2, \ldots$, where

$$\mathcal{B} = \nabla_0\left(\int_0^s(\cdot)ds\right)^2,$$

$$\nabla_0 = \frac{1}{3}\nabla^2.$$

Integrating the nonclassical angluar flux over the unit sphere we obtain

$$\varphi = \left(\sum_{n=0}^{\infty}\frac{\varepsilon^{2n}}{2n+1}(3\mathcal{B})^n\right)\left[\int_0^{\infty}(1-\varepsilon^2\kappa)p(s')\varphi(\boldsymbol{x},s')ds' + \varepsilon^2\langle s\rangle_\epsilon q\right].$$

Asymptotic Analysis

Inverting the operator on the right-hand side and once again expanding it in a power series, we get

$$\left(I - \varepsilon^2\mathcal{B} - \frac{4\varepsilon^4}{5}\mathcal{B}^2 - \frac{44\varepsilon^6}{35}\mathcal{B}^3 + O(\varepsilon^8)\right)\varphi = \int_0^\infty (1-\varepsilon^2\kappa)p(s')\varphi(\boldsymbol{x}, s')ds' + \varepsilon^2\langle s\rangle_\epsilon q.$$

The solution of this equation is

$$\varphi(\boldsymbol{x}, s) = \left(I + \varepsilon^2\frac{s^2}{2!}\nabla_0 + \frac{9\varepsilon^4}{5}\frac{s^4}{4!}\nabla_0^2 + \frac{27\varepsilon^6}{7}\frac{s^6}{6!}\nabla_0^3 + O(\varepsilon^8)\right)\phi(\boldsymbol{x}),$$

where

$$\phi(\boldsymbol{x}) = \sum_{n=0}^\infty \varepsilon^2\phi_{2n}(\boldsymbol{x}),$$

with $\phi_{2n}(\boldsymbol{x})$ undetermined at this point.

Asymptotic Analysis

We now multiply φ by $e^{-\int_0^s \Sigma_t(s')ds'} / \langle s \rangle_\epsilon$ and operate by $\int_0^\infty (\cdot) ds$. We obtain an expression for the scalar flux:

$$\Phi(\boldsymbol{x}) = \left(I + \varepsilon^2 \frac{\langle s^3 \rangle_\epsilon}{3! \langle s \rangle_\epsilon} \nabla_0 + \frac{9\varepsilon^4}{5} \frac{\langle s^5 \rangle_\epsilon}{5! \langle s \rangle_\epsilon} \nabla_0^2 + \frac{27\varepsilon^6}{7} \frac{\langle s^7 \rangle_\varepsilon}{7! \langle s \rangle_\epsilon} \nabla_0^3 + O(\varepsilon^8) \right) \phi(\boldsymbol{x}).$$

Moreover, we can write

$$\int_0^\infty p(s)\varphi(\boldsymbol{x}, s) ds = \left(\sum_{n=0}^{\infty} \varepsilon^{2n} U_n \nabla_0^n \right) \Phi(\boldsymbol{x}),$$

with $U_0 = 1;\ U_1 = \frac{\langle s^2 \rangle_\epsilon}{2!} - \frac{\langle s^3 \rangle_\epsilon}{3! \langle s \rangle_\epsilon};$

$$U_2 = \frac{9}{5} \left[\frac{\langle s^4 \rangle_\epsilon}{4!} - \frac{\langle s^5 \rangle_\epsilon}{5! \langle s \rangle_\epsilon} \right] - \frac{\langle s^3 \rangle_\epsilon}{3! \langle s \rangle_\epsilon} U_1;$$

$$U_3 = \frac{27}{7} \left[\frac{\langle s^6 \rangle_\epsilon}{6!} - \frac{\langle s^7 \rangle_\varepsilon}{7! \langle s \rangle_\epsilon} \right] - \frac{9}{5} \frac{\langle s^5 \rangle_\epsilon}{5! \langle s \rangle_\epsilon} U_1 - \frac{\langle s^3 \rangle_\epsilon}{3! \langle s \rangle_\epsilon} U_2;$$

Asymptotic Analysis

We can now rewrite the whole equation as

$$\left(\sum_{n=0}^{\infty} \varepsilon^{2n} V_n \nabla_0^n\right) \Phi(\boldsymbol{x}) = (1 - \varepsilon^2 \kappa) \left(\sum_{n=0}^{\infty} \varepsilon^{2n} U_n \nabla_0^n\right) \Phi(\boldsymbol{x}) + \varepsilon^2 \langle s \rangle_\epsilon q(\boldsymbol{x}),$$

where

$$V_0 = 1;$$

$$V_1 = -\frac{\langle s^3 \rangle_\epsilon}{3! \langle s \rangle_\epsilon} V_0;$$

$$V_2 = -\frac{9}{5} \frac{\langle s^5 \rangle_\epsilon}{5! \langle s \rangle_\epsilon} V_0 - \frac{\langle s^3 \rangle_\epsilon}{3! \langle s \rangle_\epsilon} V_1;$$

$$V_3 = -\frac{27}{7} \frac{\langle s^7 \rangle_\varepsilon}{7! \langle s \rangle_\epsilon} V_0 - \frac{9}{5} \frac{\langle s^5 \rangle_\epsilon}{5! \langle s \rangle_\epsilon} V_1 - \frac{\langle s^3 \rangle_\epsilon}{3! \langle s \rangle_\epsilon} V_2;$$

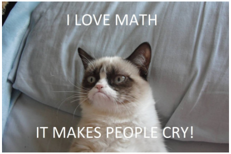
$$\dots$$

Asymptotic Analysis

Finally, we rearrange the terms and get

$$\boxed{\left(\sum_{n=0}^{\infty} \varepsilon^{2n} \left[W_{n+1}\nabla_0^{n+1} + \kappa U_n \nabla_0^n\right]\right)\Phi(\boldsymbol{x}) = \left\langle s \right\rangle_\epsilon q(\boldsymbol{x}),}$$

where $W_n = V_n - U_n$.



- If we discard the terms of $O(\varepsilon^{2n})$ in this equation, we obtain a partial differential equation for $\Phi(\boldsymbol{x})$ of order $2n$
- We will use this approach to explicitly derive the nonclassical SP_1, SP_2, and SP_3 equations
- Higher-order equations can be derived by continuing to follow the same procedure

Nonclassical Diffusion (SP_1)

Discarding the terms of $O(\varepsilon^2)$ and reverting to the original unscaled parameters, we obtain

$$-\frac{1}{6}\frac{\langle s^2\rangle}{\langle s\rangle}\nabla^2\Phi(\boldsymbol{x}) + \frac{1-c}{\langle s\rangle}\Phi(\boldsymbol{x}) = Q(\boldsymbol{x}),$$

which is the nonclassical diffusion equation.
If the free-path distribution $p(s)$ is an exponential, $\langle s^m\rangle = m!\Sigma_t^{-m}$ and this equation reduces to the classical diffusion equation

$$-\frac{1}{3\Sigma_t}\nabla^2\Phi(\boldsymbol{x}) + \Sigma_a\Phi(\boldsymbol{x}) = Q(\boldsymbol{x}).$$

Nonclassical SP_2

Discarding the terms of $O(\varepsilon^4)$ and reverting to the original unscaled parameters, we obtain

$$-\frac{1}{6}\frac{\langle s^2\rangle}{\langle s\rangle}\nabla^2\Big[\Phi(\boldsymbol{x})+\lambda_1\left[(1-c)\Phi(\boldsymbol{x})-\langle s\rangle Q(\boldsymbol{x})\right]\Big]+$$
$$\frac{1-c}{\langle s\rangle}\left[1-\beta_1(1-c)\right]\Phi(\boldsymbol{x})=\left[1-\beta_1(1-c)\right]Q(\boldsymbol{x}),$$

with $\lambda_1=\frac{3}{10}\frac{\langle s^4\rangle}{\langle s^2\rangle^2}-\frac{1}{3}\frac{\langle s^3\rangle}{\langle s\rangle\langle s^2\rangle}$ and $\beta_1=\frac{1}{3}\frac{\langle s^3\rangle}{\langle s\rangle\langle s^2\rangle}-1$.

If the free-path distribution $p(s)$ is an exponential, $\lambda_1=\frac{4}{5}$, $\beta_1=0$, and this equation reduces to the classical SP_2 equation

$$-\frac{1}{3\Sigma_t}\nabla^2\left[\Phi(\boldsymbol{x})+\frac{4}{5}\frac{\Sigma_a\Phi(\boldsymbol{x})-Q(\boldsymbol{x})}{\Sigma_t}\right]+\Sigma_a\Phi(\boldsymbol{x})=Q(\boldsymbol{x}).$$

Nonclassical SP_3

Discarding the terms of $O(\varepsilon^6)$ and reverting to the original unscaled parameters, we obtain

$$
\begin{aligned}
&-\frac{1}{6}\frac{\langle s^2\rangle}{\langle s\rangle}\nabla^2\Big[\big[1+\beta_1(1-c)\big]\Phi(\boldsymbol{x})+2\nu(\boldsymbol{x})\Big]+\frac{1-c}{\langle s\rangle}\Phi(\boldsymbol{x})=Q(\boldsymbol{x}),\\
&-\frac{1}{6}\frac{\langle s^2\rangle}{\langle s\rangle}\nabla^2\left[\frac{\lambda_1}{2}\Phi(\boldsymbol{x})+\lambda_2\nu(\boldsymbol{x})\right]+\frac{1-\beta_2(1-c)}{\langle s\rangle}\nu(\boldsymbol{x})=0,
\end{aligned}
$$

with

$$
\begin{aligned}
\lambda_2 =&\frac{1}{10\langle s^2\rangle\langle s^3\rangle-9\langle s\rangle\langle s^4\rangle}\left[\frac{9}{5}\langle s^5\rangle-\frac{27}{21}\frac{\langle s\rangle\langle s^6\rangle}{\langle s^2\rangle}+3\frac{\langle s^3\rangle\langle s^4\rangle}{\langle s^2\rangle}-\frac{10}{3}\frac{\langle s^3\rangle^2}{\langle s\rangle}\right],\\
\beta_2 =&\frac{1}{10\langle s^2\rangle_\epsilon\langle s^3\rangle_\epsilon-9\langle s\rangle_\epsilon\langle s^4\rangle_\epsilon}\left[\frac{10}{3}\frac{\langle s^3\rangle_\epsilon^2}{\langle s\rangle_\epsilon}-\frac{9}{5}\langle s^5\rangle_\epsilon\right]-1.
\end{aligned}
$$

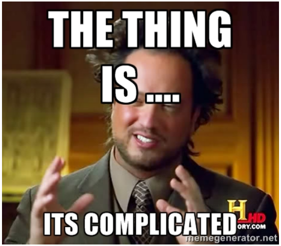
Nonclassical SP_3

If the free-path distribution $p(s)$ is an exponential, $\lambda_2 = \frac{11}{7}$, $\beta_2 = 0$, and these equations reduce to the classical SP_3 equations

$$-\frac{1}{3\Sigma_t}\nabla^2\Big[\Phi(\boldsymbol{x}) + 2\nu(\boldsymbol{x})\Big] + \Sigma_a\Phi(\boldsymbol{x}) = Q(\boldsymbol{x}),$$

$$-\frac{1}{3\Sigma_t}\nabla^2\left[\frac{2}{5}\Phi(\boldsymbol{x}) + \frac{11}{7}\nu(\boldsymbol{x})\right] + \Sigma_t\nu(\boldsymbol{x}) = 0.$$

Regarding Boundary Conditions...



- Nonclassical transport boundary conditions are not yet well-defined for the "backward" nonclassical equation
- The asymptotic analysis for the classical SP_N equations does not yield boundary conditions... and neither does the present one

Solution: manipulate the nonclassical SP_N equations into a classical form and use classical (Marshak) boundary conditions.

Nonclassical Diffusion with Vacuum Boundaries

The nonclassical diffusion equation is

$$-\frac{1}{6}\frac{\langle s^2\rangle}{\langle s\rangle}\nabla^2\Phi(\boldsymbol{x})+\frac{1-c}{\langle s\rangle}\Phi(\boldsymbol{x})=Q(\boldsymbol{x}).$$

We define

$$\widehat{\Sigma}_t=2\frac{\langle s\rangle}{\langle s^2\rangle},\qquad \widehat{\Sigma}_a=\frac{1-c}{\langle s\rangle},$$

and rewrite it as a classical diffusion equation, for which we use Marshak boundary conditions:

$$-\frac{1}{3\widehat{\Sigma}_t}\nabla^2\Phi(\boldsymbol{x})+\widehat{\Sigma}_a\Phi(\boldsymbol{x})=Q(\boldsymbol{x}),$$

$$\frac{1}{2}\Phi(\boldsymbol{x})-\frac{1}{3\widehat{\Sigma}_t}\vec{\boldsymbol{n}}\cdot\nabla\Phi(\boldsymbol{x})=0.$$

Nonclassical SP_2 with Vacuum Boundaries

$$-\frac{1}{3\widehat{\Sigma}_t}\nabla^2\widehat{\Phi}(\boldsymbol{x}) + \widehat{\Sigma}_a\widehat{\Phi}(\boldsymbol{x}) = \widehat{Q}(\boldsymbol{x}),$$
$$\frac{1}{2}\widehat{\Phi}(\boldsymbol{x}) - \frac{1}{3\widehat{\Sigma}_t}\vec{\boldsymbol{n}}\cdot\nabla\widehat{\Phi}(\boldsymbol{x}) = 0,$$

with

$$\widehat{\Sigma}_t = 2\frac{\langle s\rangle}{\langle s^2\rangle}, \qquad \widehat{\Sigma}_a = \frac{(1-c)}{\langle s\rangle}\frac{1-\beta_1(1-c)}{1+\lambda_1(1-c)},$$
$$\widehat{Q}(\boldsymbol{x}) = \frac{1-\beta_1(1-c)}{1+\lambda_1(1-c)}Q(\boldsymbol{x}), \qquad \Phi(\boldsymbol{x}) = \frac{\widehat{\Phi}(\boldsymbol{x}) + \lambda_1\langle s\rangle Q(\boldsymbol{x})}{1+\lambda_1(1-c)}.$$

Nonclassical SP_3 with Vacuum Boundaries

$$-\frac{1}{3\widehat{\Sigma}_t}\nabla^2\left[\Phi(\boldsymbol{x})+2\widehat{\Phi}_2(\boldsymbol{x})\right]+\widehat{\Sigma}_a\Phi(\boldsymbol{x})=\widehat{Q}(\boldsymbol{x}),$$

$$-\frac{1}{3\widehat{\Sigma}_t}\nabla^2\left[\frac{2}{5}\Phi(\boldsymbol{x})+\left(\frac{4}{5}+\frac{27\widehat{\Sigma}_t}{35\widehat{\Sigma}_3}\right)\widehat{\Phi}_2(\boldsymbol{x})\right]+\widehat{\Sigma}_2\widehat{\Phi}_2(\boldsymbol{x})=0,$$

$$\frac{1}{2}\Phi(\boldsymbol{x})-\frac{1}{3\widehat{\Sigma}_t}\vec{\boldsymbol{n}}\cdot\nabla\Phi(\boldsymbol{x})-\frac{2}{3\widehat{\Sigma}_t}\vec{\boldsymbol{n}}\cdot\nabla\widehat{\Phi}_2(\boldsymbol{x})+\frac{5}{8}\widehat{\Phi}_2(\boldsymbol{x})=0,$$

$$-\frac{1}{8}\Phi(\boldsymbol{x})+\frac{5}{8}\widehat{\Phi}_2(\boldsymbol{x})-\frac{3}{7\widehat{\Sigma}_3}\vec{\boldsymbol{n}}\cdot\nabla\widehat{\Phi}_2(\boldsymbol{x})=0,$$

with

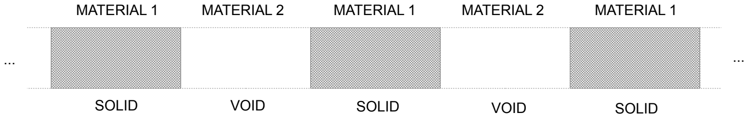
$$\widehat{\Phi}_2(\boldsymbol{x})=\frac{\nu(\boldsymbol{x})}{1+\beta_1(1-c)},\qquad \widehat{\Sigma}_t=2\frac{\langle s\rangle}{\langle s^2\rangle},$$

$$\widehat{\Sigma}_a=\frac{(1-c)}{\langle s\rangle}\frac{1}{1+\beta_1(1-c)},\qquad \widehat{Q}(\boldsymbol{x})=\frac{Q(\boldsymbol{x})}{1+\beta_1(1-c)},$$

$$\widehat{\Sigma}_2=\frac{4\left[1+\beta_1(1-c)\right]\left[1-\beta_2(1-c)\right]}{5\lambda_1\langle s\rangle},\qquad \widehat{\Sigma}_3=\frac{27}{28}\frac{\lambda_1\widehat{\Sigma}_t}{\lambda_2\left[1+\beta_1(1-c)\right]-\lambda_1}.$$

1-D random periodic media

We consider a 1-D physical system consisting of alternating layers of solid and void, periodically arranged:



- layers of material 1 and 2 have thicknesses ℓ_1 and ℓ_2, respectively; (period $\ell = \ell_1 + \ell_2$)
- the origin ($x = 0$) is *randomly placed* in the periodic system (this is equivalent to randomly placing the system in the infinite line $-\infty < x < \infty$)
- the probability P_i of finding material i in a given point x is $\ell_i/(\ell_1 + \ell_2)$

The Path-length distribution function

★ $\ell_1 < \ell_2$:

$$p(\mu,s)=\begin{cases}\frac{\Sigma_{t1}}{\ell_1}(n\ell+\ell_1-s|\mu|)e^{-\Sigma_{t1}(s-n\ell_2/|\mu|)}, & \text{if } n\ell\le s|\mu|\le n\ell+\ell_1\\ 0, & \text{if } n\ell+\ell_1\le s|\mu|\le n\ell+\ell_2\\ \frac{\Sigma_{t1}}{\ell_1}(s|\mu|-n\ell+\ell_2)e^{-\Sigma_{t1}[s-(n+1)\ell_2/|\mu|)]}, & \text{if } n\ell+\ell_2\le s|\mu|\le (n+1)\ell\end{cases}$$

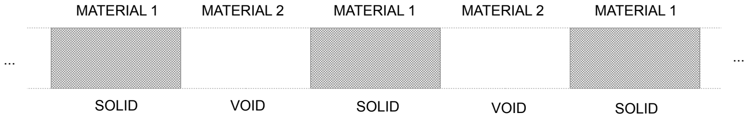
★ $\ell_1 = \ell_2$:

$$p(\mu,s)=\begin{cases}\frac{\Sigma_{t1}}{\ell_1}(n\ell+\ell_1-s|\mu|)e^{-\Sigma_{t1}(s-n\ell_2/|\mu|)}, & \text{if } n\ell\le s|\mu|\le n\ell+\ell_1\\ \frac{\Sigma_{t1}}{\ell_1}(s|\mu|-n\ell+\ell_2)e^{-\Sigma_{t1}[s-(n+1)\ell_2/|\mu|)]}, & \text{if } n\ell+\ell_2\le s|\mu|\le (n+1)\ell\end{cases}$$

★ $\ell_1 > \ell_2$:

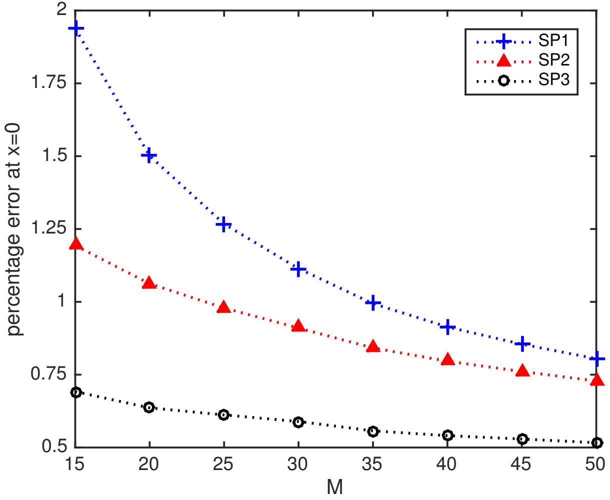
$$p(\mu,s)=\begin{cases}\frac{\Sigma_{t1}}{\ell_1}(n\ell+\ell_1-s|\mu|)e^{-\Sigma_{t1}(s-n\ell_2/|\mu|)}, & \text{if } n\ell\le s|\mu|\le n\ell+\ell_2\\ \frac{\Sigma_{t1}}{\ell_1}[(n\ell+\ell_2-s|\mu|)(1-e^{\Sigma_{t1}\ell_2/|\mu|}) \\ \qquad\qquad +\ell_1-\ell_2]e^{-\Sigma_{t1}(s-n\ell_2/|\mu|)}, & \text{if } n\ell+\ell_2\le s|\mu|\le n\ell+\ell_1\\ \frac{\Sigma_{t1}}{\ell_1}(s|\mu|-n\ell+\ell_2)e^{-\Sigma_{t1}[s-(n+1)\ell_2/|\mu|)]}, & \text{if } n\ell+\ell_1\le s|\mu|\le (n+1)\ell\end{cases}$$

1-D diffusive system



- Slab geometry
- Isotropic scattering
- Vacuum boundaries
- Isotropic source
- We define $M = \varepsilon^{-1}$, and
  - $\ell_1 = \ell_2 = 0.5 \implies \ell = 1$
  - $-M \leq x \leq M \implies \ell M = O(\varepsilon^{-1})$
  - $\Sigma_{t1} = 1 = O(1)$
  - $1 - c = 0.1 \times M^{-2} = O(\varepsilon^2)$
  - $Q_1 = 0.2 \times M^{-2} = O(\varepsilon^2)$

Error Estimates at $x = 0$



Discussion

1. The nonclassical SP_N equations provide more accurate diffusion approximations to nonclassical transport
2. However, they require all the moments of the $p(s)$ up to $2N$ to exist
3. They can be manipulated into a set of *classical* SP_N equations with modified parameters
4. Therefore, they can be implemented in already existing SP_N codes

Immediate things to do:

- We need to extend the analysis to angular dependent free-path distributions $p(\mathbf{\Omega}, s)$ (the case of slab geometry)
- We need to extend the analysis to anisotropic scattering